

Stochastic quantum dynamics beyond mean-field

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Abstract. Mean-field approaches where a complex fermionic many-body problem is replaced by an ensemble of independent particles in a self-consistent mean-field can describe many static and dynamical aspects. It generally provides a rather good approximation for the average properties of one-body degrees of freedom. However, the mean-field approximation generally fails to produce quantum fluctuations of collective motion. To overcome this difficulty, noise can be added to the mean-field theory leading to a stochastic description of the many-body problem. In the present work, we summarize recent progress in this field and discuss approaches where fluctuations have been added either to the initial time, like in the Stochastic Mean-Field theory or continuously in time as in the Stochastic Time-Dependent Hartree-Fock. In some cases, the initial problem can even be re-formulated exactly by introducing Quantum Monte-Carlo methods in real-time. The possibility to describe superfluid systems is also invoked. Successes and shortcomings of the different beyond mean-field theories are discussed and illustrated.

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Contents

1	Introduction	2	3.4	Direct in-medium two-body collisions and Extended TDHF theory	11
2	Mean-field in many-body systems	2	3.4.1	Irreversible process and Extended TDHF	12
2.1	Variational principles in closed systems	3	3.5	Summary on deterministic approaches	12
2.2	Selection of specific degrees of freedom and Ehrenfest theorem	3	4	Mean-field with initial quantum fluctuations	12
2.3	General aspects and validity of the mean-field theory	4	4.1	General strategy	13
2.4	Application of mean-field theory to the Many-Body problem	5	4.2	Stochastic Mean-Field in many-body systems	13
2.4.1	The independent particle approach for fermionic systems	5	4.3	Dispersion of one-body observable	14
2.4.2	Mean-field from variational principle	5	4.4	Adiabatic projection on collective path	15
2.4.3	Mean-field dynamics from Thouless Theorem	6	4.5	Dynamics near a saddle point: spontaneous symmetry breaking	16
2.5	Mean-field with pairing correlations	7	4.6	Stochastic Mean-Field with pairing correlations	17
2.6	Summary and discussion	8	4.7	A survey of recent applications to nuclear collisions	18
3	Dynamical Theories Beyond mean-field: a survey on deterministic approaches	8	4.7.1	Macroscopic reduction of information in mean-field dynamics	18
3.1	Limitation of the mean-field theory.	8	4.7.2	Energy dissipation	19
3.1.1	Quantum fluctuations in collective space	8	4.7.3	Nucleon exchange	20
3.1.2	departure from the single-particle (or quasi-particle) picture	9	4.8	Summary on the SMF theory	21
3.1.3	Strategy for Beyond mean-field approach to dynamics	10	5	Stochastic Schroedinger equation for N-body problems	21
3.2	General correlated dynamics: the BBGKY hierarchy	10	5.1	Stochastic process in Slater Determinant space	21
3.3	The Time-Dependent Density-Matrix Theory	11	5.1.1	Extended TDHF in the short memory approximation	22
			5.1.2	Dissipation in one-body space	22
			5.1.3	Stochastic process in one-body space	23
			5.1.4	Quantum jump for single-particle states	23
			5.2	Exact Quantum Monte-Carlo from functional integrals method	24
			5.2.1	Functional integrals for schematic residual interaction:	24
			5.2.2	General Many-Body Hamiltonian:	25

Send offprint requests to:

5.3	Quantum Monte-Carlo method for closed systems from optimal observables evolution	25
5.3.1	Link between stochastic process and observables evolution	25
5.3.2	Summary and discussion on applications	27
6	Summary	28
A	Density matrices	29
A.1	Two and three-body Correlations	29
B	Correlations between observables and Projection techniques	29
C	Mean-field as a projected dynamics	31
C.1	Projector associated to mean-field	31
D	Mean-field from Thouless theorem	31
E	Ito calculus	32
E.1	Basic rules for Ito stochastic calculation	32
E.2	Differentiation of specific operators	32
E.2.1	Entropy	32
E.3	evolution of df^{-1}	33
E.4	Evolution of a determinant	33

1 Introduction

The Time-Dependent Hartree-Fock (TDHF) or its Density Functional Theory (DFT) variant, by replacing the many-body dynamical problem of interacting particles on the dynamics of independent particle moving in an average self-consistent mean-field are certainly among the most useful tools ever to describe many facets of mesoscopic systems. Almost 50 years after its first application in nuclei [1], we have observed in the last decade a renewal of interest in the development of dynamical mean-field theories for the nuclear many-body problem [2,3,4,5,6,7]. Most advanced applications of TDHF have reached a certain level of maturity. Nowadays, calculations are performed in three dimensions without specific symmetries and including all components of the effective interaction. For a recent review, please see [8,9,10]. Recently, efforts have been made to include pairing correlations [11,12,13,14,15,16,17,18]

Despite these important progress made on the applicability of time-dependent mean-field approaches including pairing or not, it is known already from the early time of this field [19] that mean-field alone cannot describe all aspects of nuclei. Generally speaking, mean-field theory suffers from the underestimation of quantal effects in collective space and from the absence of dissipative effects induced by the coupling between single-particle degrees of freedoms (DOF) with more complex internal DOF. The former limitation is well known from nuclear structure mean-field practitioners where configuration mixing techniques are generally employed to recover the effect of quantal collective fluctuations [20,21]. Missing dissipative aspects are clearly pointed out, for instance in the context of nuclear giant resonances, where the small amplitude limit of time-dependent mean-field (RPA or QRPA) is widely used. In that case, it is well known that mean-field alone is able to describe qualitatively the mean collective energy but most often fails to

reproduce the fragmentation and damping of collective excitations [22,23].

Many theories, called hereafter beyond-mean field approaches and discussed briefly here, have been proposed to increase the predictive power of microscopic methods using the mean-field as a building block. However, most often due to the important numerical effort required, most of them have never been really applied to realistic situations. The goal of the present review is to answer to the following question:

While some effects cannot be included using the standard approach with only one mean-field trajectory, might it be possible to include some of the missing effects by considering an ensemble of mean-field trajectories, each of them being independent from the others?

A positive answer to this question is an important step, since in that case (i) the required technology is the existing one since only standard mean-field codes should be used (ii) performing several independent trajectories is possible on several independent computers that are used everyday in our scientific life. Therefore, contrary to other methods that are limited by the handling of large matrices, a stochastic approach turns out to be more practical and timely.

The present review is devoted to the description of recent progress in the field of stochastic quantum mechanic applied to the fermionic many-body problems. Depending on the physical effect that one wants to introduce beyond the mean-field, several approaches have been proposed. Some of them, like the Stochastic mean-field (SMF) are able to treat initial collective quantum fluctuations and have already been applied to realistic physical systems. Some others, most often dedicated to correlations beyond the independent particle picture that built up in time are still at the stage of formal development, requiring future efforts for practical applications.

This review is organized as follows. Basic concepts and methods associated to mean-field are first introduced. The introduction we make is oscillating between the usual academic one and arguments based on information theory. The latter is particularly useful to grasp the physical interpretation behind mean-field approaches. Deterministic approaches beyond mean-field are then briefly discussed. The rest of the review is devoted to the introduction of stochastic approaches where a correlated dynamical evolution is replaced by a set of independent particle evolutions.

2 Mean-field in many-body systems

We consider here an ensemble of N particles interacting through the following Hamiltonian

$$H = \sum_{ij} T_{ij} a_i^\dagger a_j + \frac{1}{4} \sum_{ijkl} \tilde{v}_{ijkl}^{(2)} a_i^\dagger a_j^\dagger a_l a_k + \frac{1}{36} \sum_{ijklmn} \tilde{v}_{ijklmn}^{(3)} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l + \dots, \quad (1)$$

where $\{a_i^\dagger, a_i\}$ are creation/annihilation operators associated to a complete single-particle basis. T denotes matrix

elements of the kinetic energy term while $\tilde{v}^{(2)}$ and $\tilde{v}^{(3)}$, ... correspond to fully anti-symmetric two-, three-, ... interaction matrix elements respectively.

The quantum description of such a system requires a priori the knowledge of its N -Body wave function $\Psi^*(\{\mathbf{r}_i\}, t)$ or more generally its N -body density matrix denoted by $D(\{\mathbf{r}_i\}, \{\mathbf{r}'_i\}, t)$. $\{\mathbf{r}_i\}$ is a short-hand notation for the particles coordinates $(\mathbf{r}_1, \dots, \mathbf{r}_N)$. The complexity of the Many-body problem comes from the number of degrees of freedom to consider. Except for very small number of particles, the total number of degrees of freedom to treat becomes prohibitory to get the exact ground state or the evolution of such a complex system. Therefore, we are forced to seek simplifications where much less relevant degrees of freedom are considered. The most common strategy is to assume a hierarchy between those degrees of freedom depending on their complexity. The starting point of the hierarchy consists in focusing on one-body degrees of freedom only. At the second level, one- and two-body degrees of freedom are incorporated simultaneously and so on and so forth up to the exact description.

The aim of the present section is to consider the first level. Such an approach is motivated first by the fact that most of the observations generally made on an interacting system are related to one-body quantities: deformation, collective motion... Since any one-body operator writes $O^{(1)} = \sum_{ij} \langle i|O|j \rangle a_i^\dagger a_j$, all the information on one-body properties is contained in the one-body density matrix defined as

$$\rho_{ji}^{(1)}(t) = \text{Tr}(a_i^\dagger a_j D(t)) \equiv \langle a_i^\dagger a_j \rangle. \quad (2)$$

Some properties of the one-body density as well as its connection with higher order densities are discussed in appendix A. Large effort is devoted to provide the best approximation on the one-body density only without solving the full problem. The main difficulty comes from the fact that the one-body density could not be fully isolated from other more complex degrees of freedom. Therefore by reducing the information on a closed system into a small set of variables, we are left with an open quantum system problem where this subset is coupled to the surrounding sets of irrelevant degrees of freedom.

In this chapter, variational principles are used as a starting point to discuss the reduction of information in many-body systems. Concepts like relevant/irrelevant observables, effective Hamiltonian dynamics, projections are first introduced from a rather general point of view. These concepts are then illustrated in the specific case of interacting particles.

2.1 Variational principles in closed systems

Variational principles are powerful tools to provide approximate solutions for static or dynamical properties of a system when few degrees of freedom are expected to contain the major part of the information [24, 25, 26, 27]. For time dependent problem, the Rayleigh-Ritz variational prin-

ciple generalizes as

$$S = \int_{t_0}^{t_1} dt \langle \Psi(t) | i\hbar \partial_t - H | \Psi(t) \rangle, \quad (3)$$

where S denotes the action. The action should be minimized, i.e. $\delta S = 0$ under fixed boundary conditions $|\delta \Psi(t_0)\rangle = 0$ and $\langle \delta \Psi(t_1) | = 0$. The variation has to be made on all components of the wave-function. Denoting by Ψ_i these components in a specific basis with $\Psi_i(t) = \langle i | \Psi(t) \rangle$, S becomes¹

$$\begin{aligned} S &= \int_{t_0}^{t_1} dt \sum_i \left\{ i\hbar \Psi_i^*(t) \partial_t \Psi_i(t) - \sum_j \Psi_i^*(t) H_{ij} \Psi_j(t) \right\} \\ &\equiv \int_{t_0}^{t_1} dt \left\{ i\hbar \Psi^* \partial_t \Psi - \mathcal{H}[\Psi, \Psi^*] \right\}, \\ &= \int_{t_0}^{t_1} dt \mathcal{L}[\Psi^*, \Psi, \dot{\Psi}], \end{aligned} \quad (4)$$

where $\mathcal{H}[\Psi^*, \Psi]$ and $\mathcal{L}[\Psi^*, \Psi]$ stands for the time-dependent Hamiltonian and Lagrangian respectively written in a functional form. In expression (6), a discrete basis is used. The generalization to continuous basis is straightforward. If the states $\{i\}$ do form a complete basis of the full Hilbert space relevant for the considered problem, then the minimization procedure leads to

$$\begin{cases} i\hbar \partial_t |\Psi(t)\rangle = H |\Psi(t)\rangle, \\ -i\hbar \partial_t \langle \Psi(t) | = \langle \Psi(t) | H, \end{cases} \quad (7)$$

which is nothing but the standard Schrödinger equation and its adjoint. Note that the second equation has been obtained by making variations with respect to the components Ψ_i after integrating by parts and underlines the crucial role of boundary conditions. The connection to classical equation of motion can be made using the functional form and introducing the field Φ and momenta Π coordinate such that $\Psi = (\Phi + i\Pi)/\sqrt{2}$, leading to [24]

$$\frac{\partial \Phi}{\partial t} = \frac{\partial \mathcal{H}}{\partial \Pi}, \quad \frac{\partial \Pi}{\partial t} = -\frac{\partial \mathcal{H}}{\partial \Phi}, \quad (8)$$

which are nothing but Hamilton's equations for the conjugate variables (Φ, Π) .

2.2 Selection of specific degrees of freedom and Ehrenfest theorem

The interest of variational principle is obviously not to recover the Schrödinger equation but stems from the possibility to restrict the variation to a smaller sub-space of

¹ Note that, last expression can very easily be transformed into a more symmetric and more natural form:

$$S = \int_{t_0}^{t_1} dt \mathcal{L}[\Psi^*, \Psi, \dot{\Psi}, \dot{\Psi}^*]. \quad (4)$$

the full Hilbert space and/or to a specific class of wave-functions. Then, the dynamics is not exact anymore but will be the best approximation within the selected space or trial states class.

We will consider here the important case where specific local transformations exist between any of the trial state $|\Psi\rangle$ and surrounding states. Explicitly, we consider the case:

$$|\Psi + \delta\Psi\rangle = e^{\sum_{\alpha} \delta q_{\alpha} A_{\alpha}} |\Psi\rangle, \quad (9)$$

where $\{\delta q_{\alpha}\}$ and A_{α} denotes respectively a set of parameters and operators. In most cases, the set of trial states is written as [28]

$$|\Psi(\mathbf{Q})\rangle = R(\mathbf{Q})|\Psi(0)\rangle = e^{\mathbf{Q} \cdot \mathbf{A}} |\Psi(0)\rangle \quad (10)$$

$R(\mathbf{Q})$ is an element of the Lie Group constructed from a parameters set $\mathbf{Q} \equiv \{q_{\alpha}\}$ and from its generators $\mathbf{A} \equiv \{A_{\alpha}\}$. Most often $|\Psi(0)\rangle$, is a state of the irreducible representation of the group. The most common examples are coherent states, independent particle states or quasi-particles vacuum (the two latter cases will be illustrated below). States written as in eq. (10) are implicit functionals of \mathbf{Q} , in the following, the simple notation $|\mathbf{Q}\rangle \equiv |\Psi(\mathbf{Q})\rangle$ is used. Variations with respect to the wave-function are now replaced by variations with respect to the parameters \mathbf{Q} with:

$$\begin{cases} |\delta\mathbf{Q}\rangle = \sum_{\alpha} \delta q_{\alpha} \left(\frac{\partial}{\partial q_{\alpha}} |\mathbf{Q}\rangle \right) \\ \langle \delta\mathbf{Q}| = \sum_{\alpha} \delta q_{\alpha}^*(t) \left(\frac{\partial}{\partial q_{\alpha}^*} \langle \mathbf{Q}| \right) \end{cases}, \quad (11)$$

or using the transformation (10) between trial states:

$$|\delta\mathbf{Q}\rangle = \sum_{\alpha} \delta q_{\alpha} A_{\alpha} |\mathbf{Q}\rangle \text{ and } \langle \delta\mathbf{Q}| = \langle \mathbf{Q}| \sum_{\alpha} \delta q_{\alpha}^*(t) A_{\alpha} \quad (12)$$

Using expressions (11) in the minimization, leads to the classical Euler-Lagrange equation of motion for the parameters [27]:

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_{\alpha}} = \frac{\partial \mathcal{L}}{\partial q_{\alpha}}, \quad \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_{\alpha}^*} = \frac{\partial \mathcal{L}}{\partial q_{\alpha}^*}. \quad (13)$$

If instead, expressions (12) are used, the following two equations of motion, corresponding respectively to the variations δq_{α}^* and δq_{α} , are obtained:

$$\begin{cases} i\hbar \langle \mathbf{Q}| A_{\alpha} | \dot{\mathbf{Q}} \rangle = \langle \mathbf{Q}| A_{\alpha} H | \mathbf{Q} \rangle, \\ i\hbar \langle \dot{\mathbf{Q}} | A_{\alpha} | \mathbf{Q} \rangle = -\langle \mathbf{Q}| H A_{\alpha} | \mathbf{Q} \rangle, \end{cases} \quad (14)$$

which combined together gives the evolution

$$i\hbar \frac{d\langle A_{\alpha} \rangle}{dt} = \langle [A_{\alpha}, H] \rangle. \quad (15)$$

We recognize here nothing but the Ehrenfest theorem, giving the evolution of any operator $\{A_{\alpha}\}$ with the Hamiltonian H . Therefore, starting from a density $D(t_0) = |\mathbf{Q}\rangle \langle \mathbf{Q}|$, for one time step the $\{\langle A_{\alpha} \rangle\}$ evolutions identify to the exact evolution although the state is constrained to remains in a sub-class of trial states.

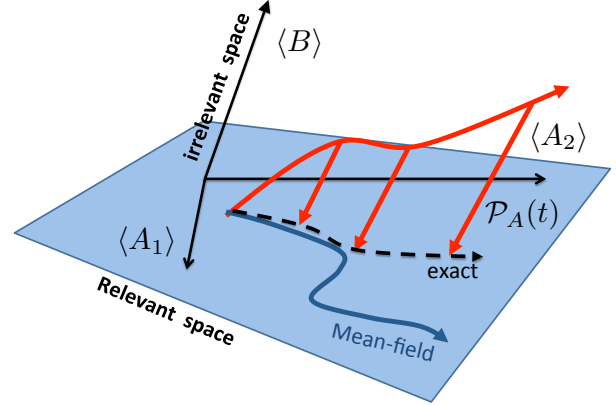


Fig. 1. (Color online) Schematic representation of the mean-field evolution. The space associated to relevant DOF, the $\{\langle A_{\alpha} \rangle\}$ is displayed by the shaded blue area, while irrelevant degrees of freedom are labelled generically by $\{\langle B \rangle\}$. Assuming, that the state is initially properly described in the relevant space, the exact dynamics escape from this space due to the coupling with irrelevant DOFs. The mean-field evolution can be seen as an approximation to the exact dynamics projected on the relevant space. This projection is expected to be perfect for short time, but will deviate from the exact projection for long time.

2.3 General aspects and validity of the mean-field theory

The mean-field concept is inherently connected to the selection of some degrees of freedom (DOF) that are assumed to be of particular relevance for the specific problem under interest. Starting from a simple trial state, the use of a variational principle insures that the $\langle A_{\alpha} \rangle$ dynamics is good over short time. Due to the specific properties of the variational space, it also lead to a closed set of the equation of motion, i.e.

$$\frac{d\langle A_{\alpha} \rangle}{dt} = \mathcal{F}(\{\langle A_{\beta} \rangle\}). \quad (16)$$

Therefore, the knowledge of the expectation values $\{\langle A_{\alpha} \rangle\}$ at initial time is sufficient to perform the long time dynamics. The functional $\mathcal{F}(\cdot)$ is generally a rather complex, most often non-linear function of the relevant DOF. The mean-field dynamics can be schematically represented as in Fig. 1 and corresponds to an approximation to the exact evolution projected on the selected DOF. Besides the schematic picture, a projector $\mathcal{P}_A(t)$ can be explicitly introduced (see appendix B and C) associated to the information carried out by the observation of relevant DOF at a given time. Then, the Hamiltonian can be separated as:

$$H = \underbrace{\mathcal{P}_A(t)H}_{H_{\text{MF}}(t)} + \underbrace{(1 - \mathcal{P}_A(t))H}_{V_{\text{res}}(t)}.$$

Then, the mean-field approximation consists in neglecting the residual interaction $V_{\text{res}}(t)$. The validity of the mean-field approximation strongly depends on the information

carried out by the observables $\{A_\alpha\}$ and on the effects of the residual part of the Hamiltonian.

If the system is allowed to explore more general variational states, the evolution a priori will not be closed in terms of the relevant degrees of freedom and will be given by:

$$\frac{d\langle A_\alpha \rangle}{dt} = \mathcal{H}(\{\langle A_\beta \rangle\}, \{\langle B_i \rangle\}) \quad (17)$$

where $\langle B_i \rangle$ is a generic notation for all degrees of freedom that are not in the $\langle A_\alpha \rangle$ space. Due to the coupling between the selected DOF and other DOF, the mean-field evolution is not expected to be valid for the long time evolution. To overcome this difficulty, it is necessary to go beyond mean-field by treating explicitly or implicitly the effect of irrelevant DOF on the set of $\{A_\alpha\}$. The end of this section illustrates applications of the mean-field theory in the context of interacting fermions while the main goal of this review is essentially devoted to general methods going Beyond Mean-Field.

2.4 Application of mean-field theory to the Many-Body problem

Notions introduced in previous section are illustrated here for the problem of N interacting particles. Our starting point is the variational principle written in this case as

$$S = \int_{t_0}^{t_1} dt \int_{\{\mathbf{r}_i\}} \left[\prod_i d^3 \mathbf{r}_i \right] \Psi^*(\{\mathbf{r}_i\}, t) \left\{ i\hbar \partial_t - H(\{\mathbf{r}_i\}) \right\} \Psi(\{\mathbf{r}_i\}, t) \quad (18)$$

where Ψ denotes a N -body wave-packets functional of the particles positions $\{\mathbf{r}_i\} \equiv (\mathbf{r}_1, \dots, \mathbf{r}_N)$. H corresponds to a Many-Body Hamiltonian given by (1). For the sake of simplicity, we will consider here two-body Hamiltonian only.

In the following, the so-called "independent particle" or "mean-field" approximation is first presented for fermions. As illustrated previously, different strategies can be employed to introduce mean-field, namely variational principle, Ehrenfest theorem, or projection leading to effective Hamiltonian. Although, strong connections exist between them, important features might be completely missed by using only one of them. For instance, the reduction of information is best seen using variational principle while missing pieces appear more clearly using the Ehrenfest theorem and/or a direct separation of the Hamiltonian into a mean-field and residual part. For this reason, different approaches are discussed below.

2.4.1 The independent particle approach for fermionic systems

If the two-body interaction is neglected in the Hamiltonian, then, the exact many-body wave-function is exactly

known and reduces to an anti-symmetric product (Slater determinant) of single-particle orthogonal states, denoted by $\{\varphi_\alpha\}$

$$\Psi(\{\mathbf{r}_i\}) = \mathcal{A}(\varphi_1(\mathbf{r}_1) \cdots \varphi_N(\mathbf{r}_N)) \quad (19)$$

where $\mathcal{A}(\cdot)$ denotes the anti-symmetrization operator. The associated one-body density matrix ρ reads

$$\rho = \sum_{\alpha=1, N} |\varphi_\alpha\rangle \langle \varphi_\alpha|. \quad (20)$$

It can be easily checked that $\text{Tr}(\rho) = N$ and $\rho^2 = \rho$ underlining that it has exactly N occupation numbers equal to one while the others equal to zero. In the following, we will use the greek notation α for occupied (hole) states. For independent particle states, correlations matrices vanish at any order and all the information on the system is contained in the one-body density matrix. This is illustrated by the fact that, for any order k , the k -body density matrix is given by an anti-symmetric product of the one-body density matrix (see appendix A):

$$\begin{aligned} \rho_{12} &= \rho_1 \rho_2 (1 - P_{12}), \\ \rho_{123} &= \rho_1 \rho_2 \rho_3 (1 - P_{12})(1 - P_{13} - P_{23}), \\ &\dots \end{aligned}$$

Here, notations of refs. [22, 29]) are used, where the indices refer to the particle on which the operator is applied. Therefore, all observables including the energy becomes a functional of the one-body density matrix components, that plays the role of the $\{\langle A_\alpha \rangle\}$ introduced previously

2.4.2 Mean-field from variational principle

When the two- (and more) body interaction is plugged in, the wave-function cannot be written in the simple form (19). However, one could still find an approximate solution by restricting the trial wave-function to a Slater determinant, this is the so-called Hartree-Fock or Time-Dependent Hartree-Fock approximation first proposed in refs. [30, 31] and [32]. In that case, the action reduces to [24]

$$S = \int_{t_0}^{t_1} ds \sum_{\alpha} \int_{\mathbf{r}} d^3 \mathbf{r} \left\{ i\hbar \varphi_{\alpha}^*(\mathbf{r}, s) \dot{\varphi}_{\alpha}^*(\mathbf{r}, s) - \mathcal{H}[\{\varphi_{\alpha}\}, \{\varphi_{\alpha}^*\}] \right\}, \quad (21)$$

where $\mathcal{H}[\{\varphi_{\alpha}\}, \{\varphi_{\alpha}^*\}]$ is given by

$$\begin{aligned} \mathcal{H}[\{\varphi_{\alpha}\}, \{\varphi_{\alpha}^*\}] &= \sum_{\alpha} \langle \varphi_{\alpha} | T | \varphi_{\alpha} \rangle \\ &+ \frac{1}{4} \sum_{\alpha, \beta} \langle \varphi_{\alpha} \varphi_{\beta} | \tilde{v}_{12} | \varphi_{\alpha} \varphi_{\beta} \rangle. \end{aligned} \quad (22)$$

Such a state can grasp part of the two-body effects through the introduction of a self-consistent mean-field. Variation

of the action (21) have to be made with respect to the components of the single-particle basis $\{\varphi_\alpha^*(\mathbf{r})\}$ or its complex conjugate $\{\varphi_\alpha(\mathbf{r})\}$ leading to

$$i\hbar \frac{\partial}{\partial t} \varphi_\alpha(\mathbf{r}) = \frac{\delta \mathcal{H}}{\delta \varphi_\alpha^*(\mathbf{r})} \text{ and } i\hbar \frac{\partial}{\partial t} \varphi_\alpha^*(\mathbf{r}) = -\frac{\delta \mathcal{H}}{\delta \varphi_\alpha(\mathbf{r})}. \quad (23)$$

Above equations of motion are generally written in terms of the mean-field Hamiltonian defined through

$$\frac{\delta \mathcal{H}}{\delta \varphi_\alpha^*} \equiv h[\rho] \varphi_\alpha \text{ with } h[\rho] = T + \text{Tr}_2 \tilde{v}_{12} \rho_2. \quad (24)$$

Here, T denotes matrix elements of the kinetic part while the second term corresponds to the average potential created by the N particles. In equation (24), $\text{Tr}_2(\cdot)$ is the partial trace on the second particle (for instance $\langle i | \text{Tr}_2 \tilde{v}_{12} \rho_2 | j \rangle = \sum_{kl} \langle ik | \tilde{v}_{12} | jl \rangle \langle l | \rho | k \rangle$). Finally, the N -body wave-function reduces to a set of coupled Schrödinger equation for occupied states (using the short-hand notation $|\varphi_\alpha\rangle = |\alpha\rangle$):

$$i\hbar \frac{d|\alpha\rangle}{dt} = h[\rho] |\alpha\rangle. \quad (25)$$

One-body density evolution: From the single-particle state evolution (23), we deduce that

$$\begin{aligned} i\hbar \partial_t \rho &= (i\hbar \partial_t |\alpha\rangle) \langle \alpha| + i\hbar \partial_t \langle \alpha| (i\hbar \partial_t |\alpha\rangle) \\ &= [h[\rho], \rho]. \end{aligned} \quad (26)$$

This equation of motion, called mean-field approximation or TDHF, represents the optimal path in the space of one-body observables for short time evolutions. Indeed, Slater determinants correspond to a specific class of trial states discussed in section 2.2. According to the Thouless theorem [33], any local transformation of a Slater determinant $|\Psi\rangle$ into another Slater determinant writes

$$|\Psi + \delta\Psi\rangle = e^{\sum_{ij} \delta Z_{ij} a_i^\dagger a_j} |\Psi\rangle. \quad (27)$$

Said differently, the set of one-body operators $\{a_i^\dagger a_j\}$ are generators of the transformation between Slater determinants. Accordingly, the variational principle automatically ensures that

$$i\hbar \frac{d}{dt} \langle a_i^\dagger a_j \rangle = \langle [a_i^\dagger a_j, H] \rangle \quad (28)$$

along the path. It could indeed be checked that the evolution of one-body observables estimated through the Ehrenfest theorem using a Slater determinant gives the mean-field evolution (26).

2.4.3 Mean-field dynamics from Thouless Theorem

Mean-field evolution corresponds to a projected dynamic onto the space of relevant one-body degrees of freedom where the coupling to irrelevant degrees of freedom (correlation) is neglected. A projected Hamiltonian could be

explicitly constructed using the projection technique introduced in section C. Here, a more direct method is used first to directly separate the Hamiltonian into a mean-field part and residual part and second to illustrate that mean-field could be obtained even without the variational principle.

To precise the missing part, we write the Slater determinant in second quantization form $|\Psi\rangle = \Pi_\alpha a_\alpha^\dagger |-\rangle$ and complete the occupied states by a set (possibly infinite) of unoccupied single-particle states (also called particle states) labeled by $\bar{\alpha}$ and associated to the creation/annihilation $a_{\bar{\alpha}}^\dagger$ and $a_{\bar{\alpha}}$. The completed basis verifies

$$\sum_\alpha |\alpha\rangle \langle \alpha| + \sum_{\bar{\alpha}} |\bar{\alpha}\rangle \langle \bar{\alpha}| \equiv \rho + (1 - \rho) = 1. \quad (29)$$

From this closure relation, any creation operator associated to a single-particle states $|i\rangle$ decomposes as

$$a_i^\dagger = \sum_\alpha a_\alpha^\dagger \langle \alpha | i \rangle + \sum_{\bar{\alpha}} a_{\bar{\alpha}}^\dagger \langle \bar{\alpha} | i \rangle. \quad (30)$$

For instance, restarting from the general expression of H and expressing the different single-particle states (i, j, k, l) in the particle-hole basis gives:

$$\begin{aligned} H |\Psi\rangle &= \left\{ -\frac{1}{2} \text{Tr}(\tilde{v}_{12} \rho_1 \rho_2) \right. \\ &+ \sum_{\alpha, \beta} \langle \beta | \rho h[\rho] | \alpha \rangle a_\beta^\dagger a_\alpha + \sum_{\bar{\alpha}, \bar{\beta}} \langle \bar{\alpha} | h[\rho] | \bar{\beta} \rangle a_{\bar{\alpha}}^\dagger a_{\bar{\beta}} \\ &\left. + \frac{1}{4} \sum_{\bar{\alpha}, \bar{\beta}, \alpha, \beta} \langle \bar{\alpha} \bar{\beta} | \tilde{v} | \alpha \beta \rangle a_{\bar{\alpha}}^\dagger a_{\bar{\beta}}^\dagger a_\beta a_\alpha \right\} |\Psi\rangle \end{aligned} \quad (31)$$

where commutations have been performed in such a way that all creation operators are on the left and where $a_{\bar{\alpha}}^\dagger |\Psi\rangle = a_{\bar{\alpha}} |\Psi\rangle = 0$ has been used. The three terms above are denoted hereafter respectively by $E_0[\rho]$, $H_{MF}[\rho]$ and $V_{res}[\rho]$.

This expression is helpful to understand the approximation made at the mean-field level. In previous section, we have shown that mean-field provides the best approximation for one-body degrees of freedom using the Ehrenfest theorem. Here, we will show that the mean-field evolution is equivalent to an effective Hamiltonian dynamics where V_{res} is neglected.

Assuming that only $E_0[\rho]$ and $H_{MF}[\rho]$ contribute to the evolution. Then, over an infinitesimal time step dt , the new state is approximated by

$$|\Psi(t + dt)\rangle \simeq \exp\left(\frac{dt}{i\hbar} E_0[\rho]\right) \exp\left(\frac{dt}{i\hbar} H_{MF}[\rho]\right) |\Psi\rangle \quad (32)$$

The first exponential is simply a global phase factor and will not contribute to observable evolution. The second contribution corresponds to an exponential of a one-body operator, which according to the Thouless Theorem [33] transforms a Slater Determinant into another Slater determinant.

Indeed, using fermionic commutation rules, gives (see appendix D)

$$\exp\left(\frac{dt}{i\hbar} H_{MF}(\rho)\right) |\Psi\rangle = \Pi_\alpha a_{\alpha+d\alpha}^\dagger |-\rangle, \quad (33)$$

where the states $|\alpha + d\alpha\rangle$ are the new single-particle states deduced from the $|\alpha\rangle$ through the mean-field evolution, Eq. (25). Besides the fact that the mean-field is directly recovered, another interest of the present approach is to provide an effective Hamiltonian that is directly separated into a relevant and irrelevant part. As shown in next chapter, an explicit expression of \hat{V}_{res} is useful to discuss the departure from a mean-field dynamics.

2.5 Mean-field with pairing correlations

Mean-field theory is sometime restricted to the approximation where the many-body wave-function is replaced by a Slater determinant state. Here, mean-field will be more generally referred to the approximation where the trial state is a quasi-particle vacuum. Slater determinants is a sub-class of quasi-particle states with occupation 1 and 0. Applying the same technique as above, leads to the Time-Dependent Hartree-Fock Bogoliubov (TDHFB) where pairing correlations can be included. In that case, the generator of transformations between quasi-particle vacua are the set of operators $\{a_i^\dagger a_j, a_i^\dagger a_j^\dagger, a_i a_j\}$.

Quasi-particle vacuum: We now consider a quasi-particle vacuum written as

$$|\Psi\rangle \sim \prod_{\alpha} \beta_{\alpha} |-\rangle, \quad (34)$$

where the $\{\beta_{\alpha}\}$ denotes a complete set of quasi-particle annihilation operators. This form automatically insures $\beta_{\alpha}|\Psi\rangle = 0$ for any α . The new quasi-particle states are defined through a specific linear combination (Bogoliubov transformation) of single-particle creation/annihilation operators $\{a_i^\dagger, a_i\}$ [20]

$$\begin{cases} \beta_{\alpha} = \sum_i U_{i\alpha}^* a_i + V_{i\alpha}^* a_i^\dagger \\ \beta_{\alpha}^\dagger = \sum_i U_{i\alpha} a_i^\dagger + V_{i\alpha} a_i. \end{cases} \quad (35)$$

where matrices U et V have specific properties to insure that new operators $\{\beta_{\alpha}, \beta_{\alpha}^\dagger\}$ verify fermionic anti-commutation rules.

The information on the system is not anymore contained only in the normal density. Indeed, one should introduce the anomalous density whose matrix elements are defined by $\kappa_{ij} = \langle a_j a_i \rangle$ (which also implies $\kappa_{ij}^* = \langle a_i^\dagger a_j^\dagger \rangle$). Latter contractions cancel out for independent particle systems. The Bogoliubov transformation (Eq. (35)) can be inverted to express the a^\dagger and a operators in terms of quasi-particles operators :

$$\begin{cases} a_i = \sum_{\alpha} U_{i\alpha} \beta_{\alpha} + V_{i\alpha}^* \beta_{\alpha}^\dagger \\ a_i^\dagger = \sum_{\alpha} V_{i\alpha} \beta_{\alpha} + U_{i\alpha}^* \beta_{\alpha}^\dagger. \end{cases} \quad (36)$$

Using these expressions in ρ et κ , we deduce

$$\rho_{ij} = \sum_{\alpha} V_{j\alpha} V_{i\alpha}^* = (V^* V^T)_{ij}, \quad \kappa_{ij} = (V^* U^T)_{ij}. \quad (37)$$

These contractions are generally presented as a generalized density matrix defined as

$$\mathcal{R} = \begin{pmatrix} \langle a_j^\dagger a_i \rangle & \langle a_j a_i \rangle \\ \langle a_j^\dagger a_i^\dagger \rangle & \langle a_j a_i^\dagger \rangle \end{pmatrix} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix}. \quad (38)$$

The new contractions make possible to treat a certain class of correlations that were neglected previously. Using the Wick theorem [20, 25], components of the associated two-body correlation matrix now read

$$\begin{aligned} \rho_{ijkl}^{(2)} = \langle ij | \rho_{12} | kl \rangle &= \langle a_k^\dagger a_l^\dagger a_j a_i \rangle \\ &= \overline{a_k^\dagger a_i} \overline{a_l^\dagger a_j} - \overline{a_k^\dagger a_j} \overline{a_l^\dagger a_i} + \overline{a_k^\dagger a_l^\dagger} \overline{a_j a_i} \\ &= \rho_{ik} \rho_{jl} - \rho_{il} \rho_{jk} + \kappa_{ij} \kappa_{kl}^*. \end{aligned} \quad (39)$$

On opposite to Slater determinants, the correlation matrix denoted by C_{12} does not a priori vanish. We further see that the HFB theory leads to separable form of the two body correlation matrix elements:

$$C_{ijkl} = \kappa_{ij} \kappa_{kl}^*. \quad (40)$$

In turn, the HFB is more complex than the HF one. For instance, the state is not anymore an eigenstate of the particle number operator. We say that the particle number symmetry $U(1)$ is explicitly broken. Fluctuations associated to the particle number $N = \sum_{\alpha} a_{\alpha}^\dagger a_{\alpha}$ now write

$$\langle N^2 \rangle - \langle N \rangle^2 = 2 \text{Tr}(\kappa \kappa^\dagger) = 2 \text{Tr}(\rho - \rho^2). \quad (41)$$

In general, this quantity is non-zero for a quasi-particle vacuum. This implies for instance that at least the particle number should be constrained in average in nuclear structure studies (this is generally done by adding a specific Lagrange multiplier to the variational principle). It is also worth to mention that in TDHFB, the expectation value $\langle N \rangle$ is a constant of motion. Therefore, no specific care of particle number is necessary in the dynamical case if it has been properly adjusted at initial time.

TDHFB Equations: Since the generators of transformation between quasi-particle states now include the $\{a_i a_j\}$ and their hermitian conjugate, minimization of the action is now equivalent to optimize associated equations of motion given by the equation of motion :

$$i\hbar \frac{d}{dt} \rho_{ji} = i\hbar \frac{d}{dt} \langle a_i^\dagger a_j \rangle = \langle [a_i^\dagger a_j, \hat{H}] \rangle, \quad (42)$$

$$i\hbar \frac{d}{dt} \kappa_{ji} = i\hbar \frac{d}{dt} \langle a_i a_j \rangle = \langle [a_i a_j, \hat{H}] \rangle. \quad (43)$$

Using the Wick theorem, the set of TDHFB coupled equations are obtained [29]:

$$i\hbar \frac{d}{dt} \rho = [h, \rho] + \kappa \Delta^* - \Delta \kappa^*, \quad (44)$$

and

$$i\hbar \frac{d}{dt} \kappa = h\kappa + \kappa h^* - \rho \Delta - \Delta \rho^* + \Delta, \quad (45)$$

where Δ denotes the pairing field:

$$\Delta_{ij} = \frac{1}{2} \sum_{kl} \tilde{v}_{ijkl} \kappa_{kl}. \quad (46)$$

Finally, using the generalized density matrix \mathcal{R} and generalized HFB Hamiltonian \mathcal{H} , defined as

$$\mathcal{H} \equiv \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}, \quad (47)$$

equations on ρ and κ can be written, in a more convenient form, as

$$i\hbar \frac{d\mathcal{R}}{dt} = [\mathcal{H}, \mathcal{R}]. \quad (48)$$

The TDHFB equation generalizes the TDHF case (Eq. (26)) by accounting for pairing effects in the dynamical evolution. There is nowadays a clear effort to extend state of the art mean-field codes by including pairing correlations [11, 12, 13, 14, 15]. Note finally that, similarly to the TDHF case, one can also directly obtain the mean-field equation with pairing by splitting the Hamiltonian into a HFB part and a residual interaction part (not shown here) [15].

2.6 Summary and discussion

In this section, basic ingredients of mean-field theory have been presented starting from a variational principle. Variational principles are very helpful to understand to what extent mean-field approximation provides an optimal description of selected degrees of freedom and can be understood as a projection of the exact dynamics on a subspace of observables.

The independent particle approximation has the great advantage to replace the exact many-body problem by a much simpler one-body problem that can most often be treated numerically. However, it is rarely used in the form presented here, i.e. starting from an Hamiltonian and performing the Hartree-Fock or the Hartree-Fock Bogoliubov approximation. The first reason is that correlations called "beyond mean-field" play an important role: direct two-body effects, pairing, quantum zero point motion in collective space. TDHFB, presented above, corresponds to one of the possible extension of mean-field able to account for pairing effects. In the next section, a description of recent advances in quantum transport theory beyond mean-field is made.

A second and more subtle difficulty is that Hartree-Fock approximation starting from the bare interaction, for instance in condensed matter or in nuclear physics, does not provide a sufficiently good approximation to serve as a starting point for the nuclear many-body problem. To overcome this difficulty, the independent particle picture is still used but in a functional spirit within the Density Functional Theory (condensed matter) or Energy Density Functional (nuclear physics) framework.

3 Dynamical Theories Beyond mean-field: a survey on deterministic approaches

In previous sections, the independent particle approximation to the N-body problem has been introduced. This approximation has played and continues to play a major role for our understanding of interacting systems. While the gross features of most nuclei are properly accounted for by replacing the complex many-body wave-function by a Slater determinant and an effective Hamiltonian (EDF), most often, physical processes reveal correlations beyond mean-field [21]. The complexity of nuclei stems from the many facets of correlations (see Figure 2). For instance short and long range correlations in static nuclei could only be accounted for by a proper treatment of pairing effects and configuration mixing. Conjointly, as collision energies between two nuclei increase, the Pauli principle becomes less effective to block direct nucleon-nucleon collisions. Then, two-body correlations should explicitly be accounted for. During the past decades, several approaches have been introduced to treat correlations beyond mean-field in a quantum theory. The development of such a theory has been strongly influenced by concepts developed for open quantum systems [34]. In that case, one-body degrees of freedom are the relevant observables and play the role of a system coupled to the surrounding environment of more complex observables. Recent advances in theories treating correlations beyond mean-field are presented here. A comprehensive list of theories introduced in this section is given in table 1, in each case the associated acronym and key observables are given.

3.1 Limitation of the mean-field theory.

Mean-field theories is attractive due to its simplicity compared to the exact treatment of a many-body problem. While this approach can grasp many phenomena, it also suffers for some drawbacks that are discussed below.

3.1.1 Quantum fluctuations in collective space

The TDHF or TDHFB approaches, discussed in previous section describe the quantal evolution of single-particles or quasi-particles. While quantal fluctuations in collective space are not strictly zero, it is clear from the Wick theorem that mean-field theory, relies on a quasi-classical approximation for quantum fluctuations in the space of relevant degrees of freedom, i.e.:

$$\frac{1}{2} (\langle A_\alpha A_\beta \rangle + \langle A_\beta A_\alpha \rangle) \approx \langle A_\alpha \rangle \langle A_\beta \rangle. \quad (49)$$

This classical approximation does not necessarily implies that mean-field alone cannot be predictive for fluctuations. Unfortunately, for nuclear systems, fluctuations are severely underestimated compared to experimental observations. This problem is rooted in the description of the system in terms of a single independent particle or quasi-particle pure state. In nuclear structure studies, zero point

Name	approximation	Quantities evolved	associated observables
TDHF	mean-field (m.-f.)	$\rho = \sum_{\alpha} \varphi_{\alpha}\rangle\langle\varphi_{\alpha} $	one-body
TDHF-Bogoliubov (TDHFB)	m.-f. + pairing	ρ, κ	generalized one-body
Beyond-Mean-Field Deterministic			
Extended-TDHF (ETDHF)	m.-f. + NN collision (dissipation)	$\rho = \sum_{\alpha} \varphi_{\alpha}\rangle n_{\alpha} \langle\varphi_{\alpha} $	one-body
Time Dept. Density Mat. (TDDM)	m.f. + two-body correlations	ρ, C_{12}	one- and two-body
TDDM ^P	m.f. + two-body correlations (approximation of TDDM focused on pairing)	ρ, C_{12}	one- and two-body
Beyond-Mean-Field Stochastic			
Stochastic mean-field (SMF)	m.-f. + initial fluctuation	$D = \overline{\Psi}\rangle\langle\overline{\Psi} $ Random Initial Value	conf. mixing
Stochastic-TDHF (STDHF)	m.-f. + NN collision (dissipation+fluctuations)	$D = \overline{\Psi}\rangle\langle\overline{\Psi} $ Quant. Jump between SD	one-body
Quantum Monte-Carlo (QMC)	Exact (within stat. errors) Quantum Jump	$D = \overline{\Psi}_1\rangle\langle\overline{\Psi}_2 $	all

Table 1. Summary of microscopic approaches presented in this document.

collective fluctuations are generally incorporated through the mixing of different configurations, this is the so-called Generator coordinate method. In transport models, as we will illustrate below, one can eventually cure this problem by incorporating DOF associated to fluctuations directly in the description.

3.1.2 departure from the single-particle (or quasi-particle) picture

Even, if the system is properly described by a pure independent particle state at initial time, it is expected that correlations beyond the mean-field will be built up in time leading to a failure of mean-field approximation for long time evolution (see also Fig. 1.). In expression (31), a clear separation is made between what is properly treated at the mean-field level ($E_0[\rho]$ and $H_{MF}[\rho]$) and what is neglected, i.e. $V_{res}[\rho]$. At this point several comments are in order:

- The validity of the mean-field approximation depends on the intensity of the residual interaction which itself

depends on the SD state $|\Phi\rangle$ and therefore will significantly depend on the physical situation. Using simple arguments [35], the time τ_{SD} over which the Slater determinant picture breaks down could be expressed as:

$$\tau_{SD} = \frac{\hbar}{2} \left(\frac{1}{N} \sum_{\bar{\alpha}\bar{\beta}\alpha\beta} |\langle\bar{\alpha}\bar{\beta}|\tilde{v}|\alpha\beta\rangle|^2 \right)^{-1/2}. \quad (50)$$

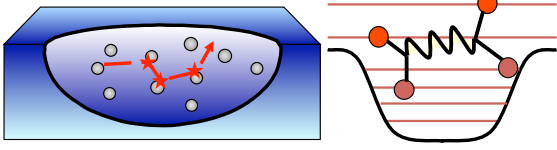
In nuclear physics, typical values of the residual interaction leads to $\tau_{SD} \simeq 100 - 200$ fm/c. Therefore, even if the starting point is given by an independent particle wave-packet, the exact evolution will deviate rather fast from the mean-field dynamics. This gives strong arguments in favor of theories beyond TDHF.

- An alternative expression of the residual interaction which is valid in any basis, is

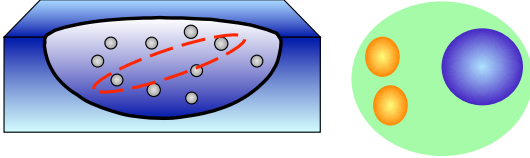
$$V_{res}[\rho] = \frac{1}{4} \sum_{ijkl} \langle ij|(1-\rho_1)(1-\rho_2)\tilde{v}_{12}\rho_1\rho_2|kl\rangle a_i^\dagger a_j^\dagger a_l a_k.$$

This expression illustrates that the residual interaction associated to a Slater determinants could be seen

In-medium nucleon-nucleon collisions



Pairing correlation



Configuration mixing (collective variables zero point motion)

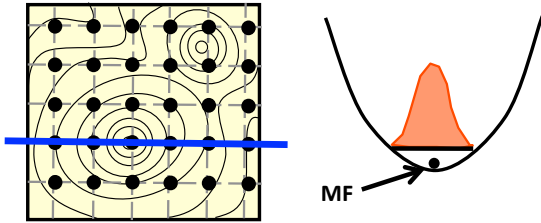


Fig. 2. Schematic illustration of the different types of correlation beyond mean-field. From top to bottom, direct in-medium nucleon-nucleon collisions, pairing and correlations associated to configuration mixing are respectively shown. Assuming that a system is properly described by a Slater determinant, direct nucleon-nucleon collisions is the first source of departure from the independent particle picture and is the physical process at the origin of thermalization. However, at low internal excitation energies, this effect is strongly hindered due to Pauli effect induced by surrounding nucleons and other correlations dominate. Pairing affects nuclear structure properties like masses, collective motion, pair transfer, ... Configuration mixing, generally incorporated through the Generator Coordinate method, tell us that nuclei could not a priori be simply described by a single Slater determinant. While the latter misses fluctuations collective space, configuration mixing incorporates it properly.

as a "dressed" interaction which properly account for Pauli principle. Physically, the residual interaction corresponds to direct nucleon-nucleon collisions between occupied states (2 holes) which could only scatter toward unoccupied states (2 particles) due to Pauli blocking. We say sometimes that the residual interaction has a 2 particles-2 holes (2p-2h) nature.

Due to the residual interaction, the exact many-body state will become a more and more complex superposition of Slater determinants during the time evolution. As stressed in the introduction, due to the complexity of the nuclear many-body problem, the exact dynamic is rarely accessible. In the following section, methods to include correlations beyond mean-field, like direct nucleon-nucleon collisions, are discussed.

3.1.3 Strategy for Beyond mean-field approach to dynamics

We have seen in previous section that the mean-field evolution can be obtained by selecting few relevant degrees of freedom. Then, these DOF are assumed to contain all the information on the system and any irrelevant DOF is assumed to be a functional of the $\{\langle A_\alpha \rangle\}$. Accordingly, the system evolution reduces to the $\langle A_\alpha \rangle$ evolution solely (see section 2):

$$\frac{d\langle A_\alpha \rangle}{dt} = \mathcal{H}(\{\langle A_\beta \rangle\}, \{\langle B_i \rangle\}) \rightarrow \mathcal{F}(\{\langle A_\beta \rangle\}).$$

The most natural way to extend mean-field dynamics is to explicitly treat the DOF $\{\langle B_i \rangle\}$ that were neglected at the mean-field level (see Fig. 1). Except in few specific cases, one cannot consider the complete space of DOF and the set of irrelevant DOF should itself be truncated. This is what is done below where for instance only one- and two-body degrees of freedom are considered. Then, Eq. (16) is complemented by a second set of equations of motion:

$$\frac{d\langle B_i \rangle}{dt} = \mathcal{G}(\{\langle A_\beta \rangle\}, \{\langle B_i \rangle\}). \quad (51)$$

The main difficulty is the number of degrees of freedom to follow in time that becomes rapidly prohibitive for practical implementation. Noting that the knowledge of expectation values of the irrelevant DOF are rarely necessary, it is sometimes possible to reduce the complexity by not considering these DOF explicitly but by treating their effect on the relevant DOF space. Then, an improved evolution of the $\{\langle A_\alpha \rangle\}$ can be found that takes the form:

$$\frac{d\langle A_\alpha \rangle}{dt} = \mathcal{F}(\{\langle A_\beta \rangle\}) + \mathcal{K}(\{\langle A_\beta \rangle\}) + \delta K(\{\langle A_\beta \rangle\}). \quad (52)$$

where $\mathcal{F}(\cdot)$ is the previous mean-field functional. $\mathcal{K}(\langle A_\beta \rangle)$ denotes the effect of coupling to irrelevant DOF inducing departure from the mean-field path, while $\delta K(\langle A_\beta \rangle)$ treats possible effect of the component $\{\langle B_i \rangle\}$ that are not properly treated in the relevant space (like initial quantum fluctuations) and that propagates within the mean-field. Eq. (52) are generally rather complex and are obtained by first integrating Eq. (51) in time and then by projecting onto the space of relevant degrees of freedom. In particular, contrary to the original mean-field, Eq. (52) might be non-local in time, i.e. the evolution at time t depends on the whole system history.

3.2 General correlated dynamics: the BBGKY hierarchy

The use of the Ehrenfest theorem (section 2.2), underlines that the mean-field theory is particularly suited to describe one-body degrees of freedom. A natural extension of mean-field consists in following explicitly two-body degrees of freedom. Considering now the Ehrenfest theorem for the one and two-body degrees of freedom leads to two

coupled equations for the one and two-body density matrix components $\rho_{ij}^{(1)} = \langle a_j^\dagger a_i \rangle$ and $\rho_{ij,kl}^{(2)} = \langle a_k^\dagger a_l^\dagger a_j a_i \rangle$

$$\begin{cases} i\hbar \frac{\partial}{\partial t} \rho_1 = [t_1, \rho_1] + \frac{1}{2} \text{Tr}_2 [\tilde{v}_{12}, \rho_{12}] \\ i\hbar \frac{\partial}{\partial t} \rho_{12} = [t_1 + t_2 + \frac{1}{2} \tilde{v}_{12}, \rho_{12}] + \frac{1}{2} \text{Tr}_3 [\tilde{v}_{13} + \tilde{v}_{23}, \rho_{123}] \end{cases} \quad (53)$$

Above equations are the first two equations of a hierarchy equations, known as the Bogolyubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy [36, 37, 38] where the three-body density evolution is also coupled to the four body density evolution and so on and so forth. Here, we will restrict to the equations on ρ_1 and ρ_{12} which have often served as the starting point to develop transport theories beyond mean-field [39, 40, 41, 22].

3.3 The Time-Dependent Density-Matrix Theory

Mean-field approximation neglects two-body and higher correlations ($C_{12} = 0$). In that case, the equations on ρ_1 reduces to TDHF. A natural extension corresponds to neglecting three-body and higher order correlations ($C_{123} = 0$)². The resulting theory where coupled equations between the one-body density ρ_1 and the two-body correlation C_{12} are followed in time are generally called Time-Dependent Density-Matrix (TDDM) theory (see for instance [39]):

$$i\hbar \frac{\partial}{\partial t} \rho_1 = [h_1[\rho], \rho_1] + \frac{1}{2} \text{Tr}_2 [\tilde{v}_{12}, C_{12}] \quad (55)$$

together with

$$\begin{aligned} i\hbar \frac{dC_{12}}{dt} = & [h[\rho]_1 + h[\rho]_2, C_{12}] \\ & + (1 - \rho_1)(1 - \rho_2) \tilde{v}_{12} \rho_1 \rho_2 - \rho_1 \rho_2 \tilde{v}_{12} (1 - \rho_1)(1 - \rho_2) \\ & + \frac{1}{2} (1 - \rho_1 - \rho_2) \tilde{v}_{12} C_{12} - \frac{1}{2} C_{12} \tilde{v}_{12} (1 - \rho_1 - \rho_2) \\ & + \frac{1}{2} \text{Tr}_3 [(\tilde{v}_{13} + \tilde{v}_{23}), \rho_1 C_{23} (1 - P_{12} - P_{13})] \\ & + \frac{1}{2} \text{Tr}_3 [(\tilde{v}_{13} + \tilde{v}_{23}), \rho_2 C_{13} (1 - P_{21} - P_{23})]. \end{aligned} \quad (56)$$

The second term in the evolution of C_{12} , denoted by B_{12} , is called the Born term. It contains the physics of direct in-medium nucleon-nucleon collisions. Comparing B_{12} and

² Introducing the permutation operator P_{12} between two particles, defined as $P_{12} |ij\rangle = |ji\rangle$. The two-body correlation matrix is given by:

$$C_{12} = \rho_{12} - \rho_1 \rho_2 (1 - P_{12}) \quad (54)$$

while the three-body correlations C_{123} reads

$$\begin{aligned} C_{123} = & \rho_{123} - \rho_1 C_{23} (1 - P_{12} - P_{13}) \\ & - \rho_2 C_{13} (1 - P_{21} - P_{23}) \\ & - \rho_3 C_{12} (1 - P_{31} - P_{32}) \\ & - \rho_1 \rho_2 \rho_3 (1 - P_{13}) (1 - P_{12} - P_{23}). \end{aligned}$$

expression (51), we see that it is directly proportional to the residual interaction. Indeed, starting from a Slater determinant ($C_{12}(t_0) = 0$), this is the only term that does not cancel out in the evolution of C_{12} over short time. In particular, it will be responsible for the departure from an independent particle picture. The third term, denoted by P_{12} has a less straightforward interpretation. For instance, it has been shown that P_{12} could be connected to pairing correlations [42]. Finally the last two terms contains higher order p-p and h-h correlations. It is finally worth mentioning that the last term could eventually be modified to better account for conservation laws (see discussion in [43]).

Applications of the TDDM theory faces two major difficulties. First, since two-body degrees of freedom are explicitly considered, huge matrices have to be treated numerically and appropriate truncation schemes should be performed. In addition, to make realistic applications to nuclei imply the use of contact interactions (Skyrme like). These interactions, which are zero range in r -space are thus of infinite range in momentum space. This unphysical behavior of the interaction is critical in practice, since during nucleon-nucleon collisions, particles will scatter to too high momentum. No clear solution to this problem exists so far in the TDDM theory [22]. Due to these difficulties, only a few applications have been carried out so far for collective vibrations [44, 45, 46, 47], and very recently for nuclear collisions [48]. Guided by the BCS approach to pairing, a simplified version of TDDM, called TDDM^P has also been proposed to account approximately for both pairing and direct nucleon-nucleon collisions in Ref. [49].

3.4 Direct in-medium two-body collisions and Extended TDHF theory

Pairing correlations become less important when the internal excitation of the system increases. Conjointly, Pauli principle is less effective to block direct nucleon-nucleon collisions. Two-body collisions are included in the Born term B_{12} in eq. (56). In the following, we only account for this term in the evolution of C_{12} [50, 51, 52, 53, 54] leading to

$$i\hbar \frac{\partial}{\partial t} C_{12} - [h_1[\rho] + h_2[\rho], C_{12}] = B_{12}. \quad (57)$$

The standard strategy to include collisions is closely related to the theory of open quantum systems [34]. Two-body correlations are interpreted as an environment for one-body degrees of freedom. To account for two-body effects without dealing directly with two-body matrices, a projection technique "a la Nakajima-Zwanzig" [34] is used. First, the correlation equation of motion is integrated from the initial time to t_0 to time t as

$$C_{12}(t) = -\frac{i}{\hbar} ds \int_{t_0}^t U_{12}(t, s) B_{12}(s) U_{12}^\dagger(t, s) + \delta C_{12}(t), \quad (58)$$

where $U_{12}(t, s)$ represents the independent particle propagation of two particles, $U_{12} = U_1 \otimes U_2$ with

$$U(t, s) = \exp\left(-\frac{i}{\hbar} \int_s^t h[\rho(t')] dt'\right). \quad (59)$$

In expression (58), the first term represents correlations due to the residual interaction during the time interval. The second term describes propagation of the initial correlations $C_{12}(t_0)$ from t_0 to t , i.e.

$$\delta C_{12}(t) = U_{12}(t, t_0) C_{12}(t_0) U_{12}^\dagger(t, t_0). \quad (60)$$

Reporting this expression in the evolution of ρ_1 , a generalization of TDHF theory is obtained (where we omit the indice "1" in ρ_1)

$$i\hbar \frac{\partial}{\partial t} \rho = [h[\rho], \rho] + K[\rho] + \delta K(t). \quad (61)$$

Two additional terms appear compared to the original mean-field transport theory. $K[\rho]$, called collision term, reads

$$K[\rho] = -\frac{i}{\hbar} \int_{t_0}^t ds \text{Tr}_2[v_{12}, U_{12}(t, s) B_{12}(s) U_{12}^\dagger(t, s)], \quad (62)$$

and contains the effect of direct in medium collisions on the evolution of one-body degrees of freedom. As we will see below, this term is anticipated to be responsible for dissipative aspects leading eventually to the onset of thermalization in the interacting system.

The second term corresponds to the effect of initial correlations propagated through the mean-field and that will induce deviations from the mean-field picture. It can be written in a compact form as $\delta K(t)$ and is given by:

$$\delta K(t) = \text{Tr}_2[v_{12}, \delta C_{12}(t)]. \quad (63)$$

This term depends on the initial conditions considered and will be the subject of the next chapter. We should note that Eq.(61) has been introduced in the semi-classical limit in Ref.[55]. In this equation the initial correlation term $\delta K(t)$ is treated as the stochastic part of the collision term. This approach is referred to as the Boltzmann-Langevin model. For further details please see Ref.[41, 56].

3.4.1 Irreversible process and Extended TDHF

Let us first illustrate the advantages of the introduction of collision term on top of the mean-field dynamics and neglect initial correlations, i.e. $\delta K[\rho] = 0$. The resulting theory is called Extended TDHF with a non-Markovian collision term (or with "memory effects"). The terminology "non-Markovian" (in opposition to "Markovian") comes from the fact that the system at time t depends not only on the density at time t but also on its full history due to the presence of a time integral in Eq. (62).

Extended TDHF has rarely been directly applied because of the numerical effort required. In order to illustrate

these difficulties, let us introduce the single-particle basis $|\alpha(t)\rangle$ that diagonalizes the one body density $\rho_1(t)$ at a given time:

$$\rho(t) = \sum |\alpha(t)\rangle n_\alpha(t) \langle \alpha(t)|. \quad (64)$$

This basis explicitly depends on time and will be called "natural" basis or "canonical" basis hereafter. As we do expect from nucleon-nucleon collisions, the collision term induces a mixing of single-particle degrees of freedom during time evolution. Using the weak coupling approximation in combination with the first order perturbation theory, the ETDHF equation can be transformed into a generalized master equation for occupation numbers which account for the Pauli principle :

$$\frac{d}{dt} n_\alpha(t) = \int_{t_0}^t ds \{ (1 - n_\alpha(s)) \mathcal{W}_\alpha^+(t, s) - n_\alpha(s) \mathcal{W}_\alpha^-(t, s) \}. \quad (65)$$

Here, the explicit form of the gain \mathcal{W}_α^+ and loss \mathcal{W}_α^- kernels could be found in ref. [57]. Therefore, in contrast to TDHF where occupation numbers are constant during the time evolution, in ETDHF the n_α evolve and can eventually relax toward equilibrium. Such a relaxation is the only way to properly account for the thermalization process in nuclei. In ref. [57], the inclusion of correlation with Extended TDHF has been successfully tested in the simple case of two interacting nucleons in one dimension where the exact solution can also be obtained.

3.5 Summary on deterministic approaches

The aim of the present section was to give an overview of deterministic approaches that goes beyond the mean-field approximation. Among the approaches, some of them are explicitly introducing additional degrees of freedoms to follow in time, like in the TDDM case while others try to projected the effect of correlations on relevant degrees of freedom keeping only the information of the one-body density. In all cases, the level of complexity is significantly enhanced compared to mean-field and most often, application to realistic situations becomes very difficult if not impossible. In the rest of this review article, we present alternative methods based on stochastic quantum mechanics to describe either initial correlations effect or correlations that built up in time.

4 Mean-field with initial quantum fluctuations

TDHF or Extended TDHF provide approximate solutions of the N-body problem starting from a well-defined initial state and leading to a unique final state. These approaches are appropriate to describe mean values of one-body observables but generally misses fluctuations in collective space. To treat the quantum zero point motion in collective space, one can for instance account for configuration mixing through the so-called Time-Dependent

Generator Coordinate Method (TDGCM) [20, 58, 59, 60]. Such approach that keeps the full quantum coherence in collective space, is however rather involved numerically [61] and is nowadays restricted to system close to the adiabatic limit suited for rather small internal excitation. To approximately treat both quantal zero-point fluctuations and possible thermal statistical fluctuations, a stochastic scheme, called hereafter Stochastic Mean-Field (SMF) theory, has been proposed in ref. [62].

4.1 General strategy

The Stochastic Mean-Field approach starts from the hypothesis that a quantum dynamical problem can be sometimes replaced by a superposition of classical evolutions with properly chosen initial conditions. Such a replacement can even be exact in some cases [63, 64]. To focus on the main hypothesis of the SMF approach, let us consider a quantum system described by a set of degrees of freedom. To make connection with section 2, we assume that we are interested in a subset of DOF associated with the set of operators $\{A_\alpha\}$. Knowing the wave-function or more generally the density matrix $D(t_0)$, at initial time, one can estimate the expectation values of the DOF as well as associated quantal fluctuations:

$$\begin{aligned}\langle A_\alpha \rangle(t_0) &= \text{Tr}(A_\alpha D(t_0)), \\ \sigma_{\alpha\beta}(t_0) &= \frac{1}{2}(\langle A_\alpha A_\beta + A_\beta A_\alpha \rangle - \langle A_\alpha \rangle \langle A_\beta \rangle).\end{aligned}$$

As discussed previously, the exact evolution of the system requires a priori to solve the exact Liouville-von Neumann equation for $D(t)$ and can lead to rather complex coupling between relevant and irrelevant degrees of freedom. The mean-field approximation provides a simple way to focus on the mean-values $\{\langle A_\alpha \rangle\}$ but generally fails to reproduce quantum fluctuations due to its quasi-classical nature.

The Stochastic Mean-Field (SMF) approach provides an approximate way to also treat fluctuations keeping the simplicity of mean-field equation of motion. In this approach, a statistical ensemble of initial values for the $\{A_\alpha^{(n)}(t_0)\}$ are considered. Here, the label (n) refers to a sample of the statistical ensemble. This variables are now considered as classical variables whose initial statistical properties are chosen in such a way to reproduce quantum mean-values and fluctuations, i.e.:

$$\begin{aligned}\overline{A_\alpha^{(n)}(t_0)} &= \langle A_\alpha \rangle(t_0), \\ \overline{A_\alpha^{(n)}(t_0) A_\beta^{(n)}(t_0)} - \overline{A_\alpha^{(n)}(t_0)} \overline{A_\beta^{(n)}(t_0)} &= \sigma_{\alpha\beta}(t_0),\end{aligned}\quad (66)$$

where the average $\overline{X^{(n)}}$ corresponds to the classical average over different samples. Then, each initial configuration is evolved according to the classical equation of motion:

$$\frac{dA_\alpha^{(n)}}{dt} = \mathcal{F}(\{A_\beta^{(n)}\}). \quad (67)$$

In a many-body problem, the mean-field equation can be regarded as the quasi-classical approximation. As we

will see, using the SMF technique in combination with the mean-field equation of motion is a powerful tool not only to improve the description of fluctuations but also to treat the effect of fluctuations on one-body DOF. This approach, contrary to other stochastic methods, have the specificity that fluctuations are introduced at initial time only. Then, each initial condition is propagated with its own mean-field.

4.2 Stochastic Mean-Field in many-body systems

Let us consider the situation where the initial state is properly described either by a Slater determinant or a statistical ensemble of independent particles with density of the form:

$$\hat{D} = \frac{1}{z} \exp \left(\sum \lambda_i a_i^\dagger a_i \right). \quad (68)$$

where z is a normalization factor while (a_i^\dagger, a_i) are the creation/annihilation operators associated to the canonical basis $|\Phi_i\rangle$. Accordingly, its initial one-body density matrix is given by

$$\rho(t_0) = \sum_i |\Phi_i(t_0)\rangle n_i \langle \Phi_i(t_0)|. \quad (69)$$

As we have discussed in section 2, the mean-field approximation focus on the evolution of the one-body DOF only, Eq. (26) that could be simulated using the set of single-particle states Schrodinger equation:

$$i\hbar \frac{\partial}{\partial t} |\Phi_i(t)\rangle = h(\rho) |\Phi_i(t)\rangle, \quad (70)$$

while keeping the occupation number n_i constant in time.

The mean-field theory is a quantal approach and even if it usually underestimates fluctuations of collective observables in the nuclear physics context, these fluctuations are non-zero. Within mean-field theory, the expectation value of an observable \hat{A} is obtained through $\langle \hat{A} \rangle = \text{Tr}(\hat{A} \hat{D})$ where \hat{D} has the form (68). Accordingly, the quantal average and fluctuation of a one-body observable \hat{A} along the mean-field trajectory are given by:

$$\langle \hat{A} \rangle = \sum_i \langle \Phi_i(t) | \hat{A} | \Phi_i(t) \rangle n_i \quad (71)$$

and

$$\begin{aligned}\sigma_A^2(t) &= \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2 \\ &= \sum_{ij} |\langle \Phi_i(t) | \hat{A} | \Phi_j(t) \rangle|^2 n_i (1 - n_j).\end{aligned}\quad (72)$$

Let us now apply the general SMF strategy described above. We are interested here in describing one-body DOF that we will treat as classical objects with initial fluctuations. Since the knowledge of one-body DOF is equivalent to the knowledge of the density matrix ρ , we can directly consider the density matrix itself classically. Therefore a

set of initial density matrix, labelled by $\rho^{(n)}$ are considered. The initial fluctuations should be chosen in such a way that the average properties and fluctuations of one-body observables identify with the quantal expectations given by Eqs. (71) and (72) at $t = t_0$. It has been shown in ref. [62] that the matrix elements $\rho_{ij}^{(n)}$ in the complete basis $\{\Phi_i(t_0)\}$ can be taken as uncorrelated Gaussian numbers with mean values equal to

$$\overline{\rho_{ij}^{(n)}} = \delta_{ij} n_j \quad (73)$$

while their variances are determined as,

$$\overline{\rho_{ij}^{(n)} \rho_{j'i'}^{(n)}} = \frac{1}{2} \delta_{jj'} \delta_{ii'} [n_i(1 - n_j) + n_j(1 - n_i)]. \quad (74)$$

Considering the observable \hat{A} , within SMF, for a given event, its value at initial time is a fluctuating quantity given by:

$$A^{(n)}(t_0) = \sum_{ij} \langle \Phi_i(t_0) | \hat{A} | \Phi_j(t_0) \rangle \rho_{ji}^{(n)}. \quad (75)$$

An important aspect in SMF, already mentioned previously, is that both mean-values and fluctuations are obtained by performing classical average on the initial sampling. This gives:

$$\begin{aligned} \overline{A^{(n)}(t_0)} &= \sum_{ij} \langle \Phi_i(t_0) | \hat{A} | \Phi_j(t_0) \rangle \overline{\rho_{ji}^{(n)}} \\ &= \sum_i \langle \Phi_i(t_0) | \hat{A} | \Phi_i(t_0) \rangle n_i(t_0). \end{aligned}$$

Introducing $\delta A^{(n)} = A^{(n)} - \overline{A^{(n)}}$, we also have (omitting t_0 in the first line):

$$\begin{aligned} \overline{\delta A^{(n)}(t_0) \delta A^{(n)}(t_0)} &= \sum_{ijkl} \langle \Phi_i | \hat{A} | \Phi_j \rangle \langle \Phi_k | \hat{A} | \Phi_l \rangle \overline{\rho_{ji}^{(n)} \rho_{lk}^{(n)}}, \\ &= \sum_{ij} |\langle \Phi_i(t_0) | \hat{A} | \Phi_j(t_0) \rangle|^2 n_i(1 - n_j), \end{aligned}$$

proving that the classical average identifies with the quantal average, Eq. (72) at t_0

In SMF, each initial condition is evolved in time using its self-consistent mean-field equation of motion that is obtained simply by replacing ρ by $\rho^{(n)}$ in Eq. (26). For a given event, the equation of motion then reads

$$i\hbar \frac{\partial}{\partial t} \rho^{(n)}(t) = [h(\rho^{(n)}), \rho^{(n)}(t)] \quad (76)$$

with the initial condition $\rho^{(n)}(t_0) = \sum_{ij} |\Phi_i(t_0)\rangle \rho_{ij}^{(n)} \langle \Phi_j(t_0)|$. Note that, trajectories are independent from each others.

It can be shown without any difficulty that the density along each path can be written as

$$\rho^{(n)}(t) = \sum_{ij} |\Phi_i^*(t; n)\rangle \rho_{ij}^{(n)} \langle \Phi_j(t; n)|, \quad (77)$$

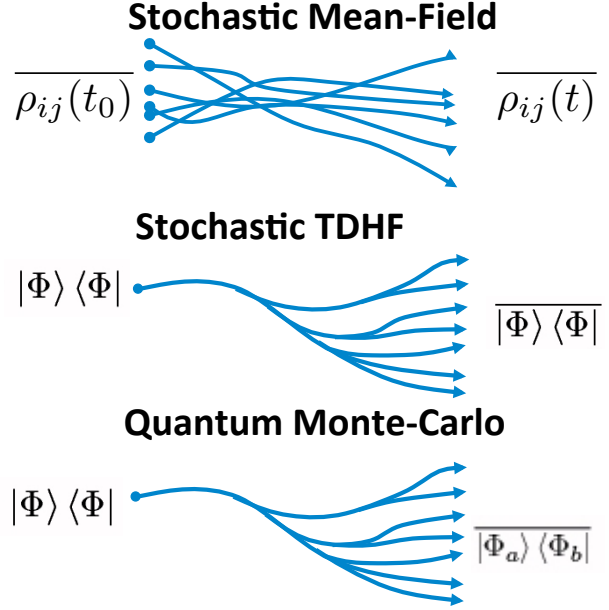


Fig. 3. Illustration of the different types of stochastic theories introduced in this section. Top: The Stochastic Mean-Field theory is introduced to account for the effect of possible initial correlation and treat fluctuations beyond the mean-field approximation. In that case, a statistical ensemble of initial densities is chosen and each set of initial values evolves independently from the others according to the quasi-classical mean-field equation. Middle: In the Stochastic TDHF theory, a random noise is introduced at each time step. This noise induces quantum jumps between densities of pure Slater determinants states. By averaging over different trajectories, the effect of two-body collisions on one-body density evolution is incorporated similarly to the Extended TDHF theory. Bottom: In the Quantum Monte-Carlo approach, all two-body correlations are a priori treated. In that case, starting from an initial independent particle state, the evolution is replaced by an ensemble of stochastic density evolutions each being written as a dyadic of Slater determinants $D = |\Phi_a\rangle \langle \Phi_b|$. The exact evolution is expected to be recovered by averaging over the dyadic.

where the matrix elements $\rho_{ij}^{(n)}$ are kept fixed in time while the single-particle wave-functions evolve according to the Schrodinger equation

$$i\hbar \frac{\partial}{\partial t} |\Phi_i(t; n)\rangle = h(\rho^{(n)}) |\Phi_i(t; n)\rangle, \quad (78)$$

with the constraint $|\Phi_i(t_0; n)\rangle = |\Phi_i(t_0)\rangle$. Note that, even if the single-particle states are identical at initial time from one event to the other, this will not be the case for $t > t_0$ due to the self-consistency of the mean-field.

4.3 Dispersion of one-body observable

As a first demonstration, we illustrate that for small amplitude fluctuations the SMF approach gives the same result for dispersion of one-body observable as the one de-

duced by Balian-Vénéroni (BV) using a variational formulation. The fluctuating part of a one body observable \hat{Q} in an event is determined by,

$$\delta Q^{(n)}(t) = \sum_{ij} \langle \Phi_j(t; n) | \hat{Q} | \Phi_i(t; n) \rangle \delta \rho_{ij}^{(n)}(t) \quad (79)$$

where $\delta \rho^{(n)}(t)$ denotes the single-particle density matrix, $\rho^{(n)}(t) = \rho(t) + \delta \rho^{(n)}(t)$ fluctuations. In order to calculate the variance of a one-body observable, we consider small amplitude fluctuations. Small fluctuations of the density matrix is determined by the time-dependent RPA equation, which is obtained by linearizing the stochastic TDHF Eq. (76) around the average evolution. As a result, the expectation value of the one-body observable can be expressed as

$$\delta Q^{(n)}(t_1) = \sum_{ij} \langle \Phi_i(t_0) | B(t_0) | \Phi_j(t_0) \rangle \delta \rho_{ji}^{(n)}(t_0) \quad (80)$$

where t_1 represents the final time at which the observation is made and t_0 is the initial time. The one-body operator $B(t)$ is defined according to

$$B_{ji}(t) = \sum_{kl} Q_{lk} \left\langle kj \left| \exp \left[-\frac{i}{\hbar} \int_t^{t_1} R(s) ds \right] \right| li \right\rangle. \quad (81)$$

where $R(t)$ is the linearized Liouville matrix obtained from the linearized TDHF equation. It is easy to show that time evolution of the one-body operator $B(t)$ is determined by the dual of the time-dependent RPA according to [62],

$$i\hbar \frac{\partial}{\partial t} B(t) = [h(\rho), B(t)] + \text{Tr} \left(\frac{\partial h}{\partial \rho} \right) \cdot [B(t), \rho].$$

The solution is determined by backward evolution with the boundary condition $B(t_1) = Q$. Then, the variance of the observable is calculated as,

$$\sigma_Q^2(t_1) = \sum |\langle \Phi_i(t_0) | B(t_0) | \Phi_j(t_0) \rangle|^2 n_i(1 - n_j). \quad (82)$$

This result is identical with the formula derived from the Balian-Vénéroni principle assuming that the deviation from the mean-field trajectory is small [65].

4.4 Adiabatic projection on collective path

In order to illustrate the fact that the SMF equation describes the dynamics of fluctuations in accordance with the one-body dissipation mechanism, we give another example in this section. We consider that the collective motion is slow and can be described by a few relevant collective variables. For example, in induced fission, collective variables maybe taken as the relative distance of fragments, mass-asymmetry and deformation parameters. Here, we consider a single collective variable $q(t)$, and introduce the quasi-static single-particle representation,

$$h(q)\Psi_j(\mathbf{r}; q) = \epsilon_j(q)\Psi_j(\mathbf{r}; q), \quad (83)$$

where $h(q) = h[\rho(q)]$ denotes the mean-field Hamiltonian, in which the time dependence of the local density $\rho(\mathbf{r}, \mathbf{r}; t)$ is parameterized in terms of the collective variable in a suitable manner. We expand the single-particle density in terms of the single-particle representation,

$$\rho(\mathbf{r}, \mathbf{r}'; t) = \sum_{kl} \Psi_k^*(\mathbf{r}; q) \rho_{kl}(t) \Psi_l(\mathbf{r}'; q). \quad (84)$$

Both the elements of density matrix $\rho_{kl}(t)$ and collective variable $q(t)$ are fluctuating quantities. In this section for clarity of notation, we ignore the event label n on these quantities. We determine the matrix elements of density in the lowest order perturbation theory in dynamical coupling $\langle \Psi_k | \partial \Psi_l / \partial q \rangle \dot{q}(t)$. It is preferable that the wave functions are close to diabatic structure. Since in the diabatic representation, dynamical coupling is expected to be small, hence, it can be treated in the weak-coupling approximation. Diabatic single-particle representation can approximately be constructed by ignoring small symmetry breaking terms in the mean-field potential [66, 67].

In order to determine the temporal evolution of collective variable, we use the total energy conservation,

$$E = \sum_{lk} \langle \Psi_k(q) | T | \Psi_l(q) \rangle \rho_{lk}(t) + \frac{1}{2} \sum_{ijkl} \rho_{ji}(t) \langle \Psi_k(q) \Psi_i(q) | V | \Psi_l(q) \Psi_j(q) \rangle \rho_{lk}(t).$$

In the many-body Hamiltonian, for simplicity we take an effective two-body interaction potential energy V . The total energy depends on time implicitly via collective variable $q(t)$ and explicitly via matrix elements $\rho_{lk}(t)$. Energy conservation requires,

$$\frac{dE}{dt} = \dot{q} \frac{\partial E}{\partial q} + \frac{\partial E}{\partial t} = 0 \quad (85)$$

In this expression $-\partial E / \partial q$ represents a dynamical force acting on the collective variable. The force depends on time, and it evolves from an initial diabatic form accompanied with deformation of Fermi surface towards an adiabatic limit associated with the adiabatic potential energy. The second term represents the rate of change of the energy due to explicit time dependence,

$$\begin{aligned} \frac{\partial E}{\partial t} &= \sum_{lk} \langle \Psi_k(q) | h(\rho) | \Psi_l(q) \rangle \frac{\partial}{\partial t} \rho_{lk}(t) \\ &= \sum_k \epsilon_k(q) \frac{\partial}{\partial t} n_k(t). \end{aligned} \quad (86)$$

Here, $n_k(t) = \rho_{kk}(t)$ represents the occupation factors of the quasi-static single-particle states. It is possible to derive a master equation for the occupation factors by substituting the expansion Eq. (84) into Eq. (76). The collision term in the master equation involves memory effects. In weak-coupling limit, the memory time of the collision kernel is determined by the correlation time of the coupling matrix elements defined as $\tau_c = \hbar / \Delta$, where Δ is

the energy range of the form factor of the coupling matrix elements. For slow collective motion, we can neglect the memory effects and carry out an expansion in powers of $t-t_1$, as it was done in the linear response treatment of ref. [68]. On the other hand, in a parabolic potential approximation of collective potential energy, it is possible to take approximately the memory effect into account by incorporating harmonic propagation of collective motion during short time intervals. In Eq. (86) factoring out $\dot{q}(t)$ from each term, it is possible to deduce a generalized Langevin equation of motion for the collective variable [69,70],

$$M\ddot{q} + \frac{1}{2} \frac{dM}{dq} \dot{q}^2 + \frac{\partial E}{\partial q} = -\gamma \dot{q} + \xi(t) \quad (87)$$

where M , γ and ξ denotes the inertia, the friction coefficient and the stochastic force, respectively. Expressions for these quantities is given in [62]. As a result of stochastic properties of the initial correlations, stochastic force has a Gaussian distribution with zero mean $\bar{\xi}(t) = 0$, and a second moment which can be expressed as,

$$\overline{\xi(t)\xi(t_1)} = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t_1)} \hbar\omega \coth \frac{\hbar\omega}{2T} \gamma(\omega) \quad (88)$$

Here $\gamma(\omega)$ denotes frequency dependent friction coefficient. This result represents the quantum fluctuation-dissipation relation associated with the one-body dissipation mechanism and it naturally emerges from the stochastic approach presented here [71,72].

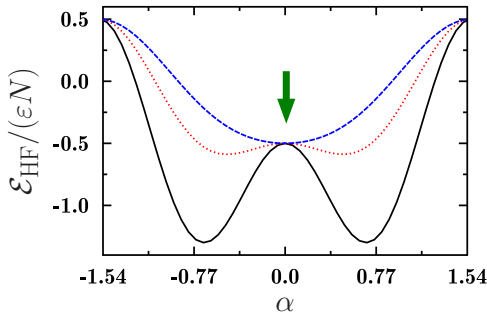


Fig. 4. (color online). Evolution of the Hartree-Fock energy \mathcal{E}_{HF} as a function of α for $\chi = 0.5$ (dashed line), $\chi = 1.8$ (dotted line) and $\chi = 5$ (solid line) for $N = 40$ particles. The arrow indicates the initial condition used in the SMF dynamics (From ref. [73]).

4.5 Dynamics near a saddle point: spontaneous symmetry breaking

As mentioned in the introduction, the mean-field theory alone cannot break a symmetry by itself. The symmetry breaking can often be regarded as the presence of a saddle point in a collective space while the absence of symmetry breaking in mean-field just means that the system will stay

at the top of the saddle point if it is there initially. Such situation is well illustrated in the Lipkin-Meshkov-Glick model. This model consists of N particles distributed in two N -fold degenerated single-particle states separated by an energy ε . The associated Hamiltonian is given by (taking $\hbar = 1$),

$$H = \varepsilon J_z - V(J_x^2 - J_y^2), \quad (89)$$

where V denotes the interaction strength while J_i ($i = x, y, z$), are the quasi-spin operators defined as

$$J_z = \frac{1}{2} \sum_{p=1}^N (c_{+,p}^\dagger c_{+,p} - c_{-,p}^\dagger c_{-,p}),$$

$$J_x = \frac{1}{2} (J_+ + J_-), \quad J_y = \frac{1}{2i} (J_+ - J_-) \quad (90)$$

with $J_+ = \sum_{p=1}^N c_{+,p}^\dagger c_{-,p}$, $J_- = J_+^\dagger$ and where $c_{+,p}^\dagger$ and $c_{-,p}^\dagger$ are creation operators associated with the upper and lower single-particle levels. In the following, energies and times are given in ε and \hbar/ε units respectively.

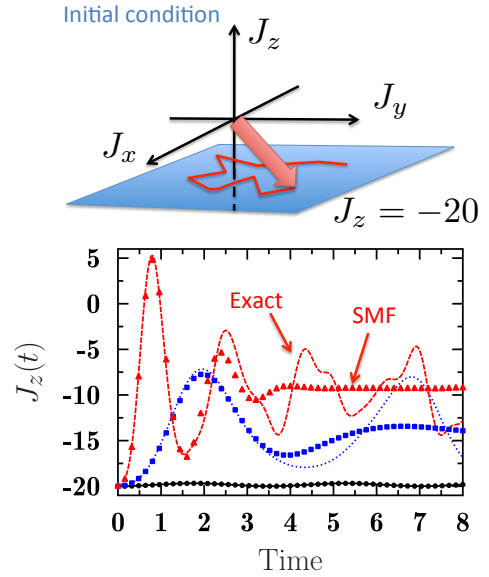


Fig. 5. (color online) Top: illustration of the initial sampling used for the SMF theory in the collective space of quasi-spins. Bottom: Exact evolution of the z quasi-spin component obtained when the initial state is $|j, -j\rangle$ for three different values of χ : $\chi = 0.5$ (solid line), $\chi = 1.8$ (dotted line) and $\chi = 5.0$ (dashed line) for $N = 40$ particles. The corresponding results obtained with the SMF simulations are shown with circles, squares and triangles respectively (adapted from [73]).

It can be shown that the TDHF dynamic can be recast as a set of coupled equations between the expectation values of the quasi-spin operators $j_i \equiv \langle J_i \rangle / N$ (for $i = x,$

y and z) given by:

$$\frac{d}{dt} \begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = \varepsilon \begin{pmatrix} 0 & -1 + \chi j_z & \chi j_y \\ 1 + \chi j_z & 0 & \chi j_x \\ -2\chi j_y & -2\chi j_x & 0 \end{pmatrix} \begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} \quad (91)$$

where $\chi = V(N-1)/\varepsilon$. Note that, this equation of motion is nothing but a special case of eq. (26) where the information is contained in the three quasi-spin components. To illustrate the symmetry breaking in this model it is convenient to display the Hartree-Fock energy \mathcal{E}_{HF} as a function of the j_z component (Fig. 4). Note that, here the order parameter $\alpha = \frac{1}{2}\arccos(-2j_z)$ is used for convenience. When the strength parameter is larger than a critical value ($\chi > 1$), the parity symmetry is broken in α direction. For $\chi > 1$, if the system is initially at the position indicated by the arrow in Fig. 4, with TDHF it will remain at this point, i.e. this initial condition is a stationary solution of Eq. (91).

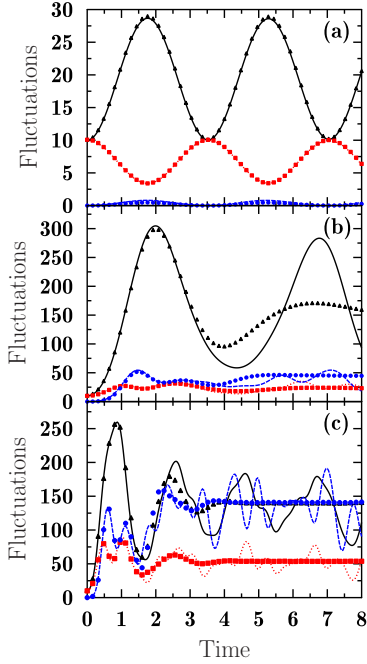


Fig. 6. (color online) Exact evolution of dispersions of quasi-spin operators obtained when the initial state is $|j, -j\rangle$ for three different values of χ , from top to bottom $\chi = 0.5$ (a), $\chi = 1.8$ (b) and $\chi = 5.0$ (c) are shown. In each case, solid, dashed and dotted lines correspond to fluctuations of each quasi-spin projection $\sigma_x^2(t)$, $\sigma_y^2(t)$ and $\sigma_z^2(t)$, respectively. In each case, results of the SMF simulations are shown with triangles (σ_x^2), squares (σ_y^2) and circles (σ_z^2). (taken from [73]).

Following the strategy discussed above, a SMF approach can be directly formulated in collective space where initial random conditions for the spin components are taken. Starting from the statistical properties (73) and (74), it can be shown that the quasi-spins should be initially sampled according to Gaussian probabilities with first mo-

ments given by [73]:

$$\overline{j_x^\lambda(t_0)} = \overline{j_y^\lambda(t_0)} = 0, \quad (92)$$

and second moments determined by,

$$\overline{j_x^\lambda(t_0)j_x^\lambda(t_0)} = \overline{j_y^\lambda(t_0)j_y^\lambda(t_0)} = \frac{1}{4N}. \quad (93)$$

while the z component is a non fluctuating quantity.

An illustration of the initial sampling (top) and of results obtained by averaging mean-field trajectories with different initial conditions is shown in Fig. 5 and compared to the exact dynamic. As we can see from the figure, while the original mean-field gives constant quasi-spins as a function of time, the SMF approach greatly improves the dynamics and follows the exact evolution up to a certain time that depends on the interaction strength. As shown in Fig. 6, the stochastic approach not only improves the description of the mean-value of one-body observables but also the fluctuations. It is finally worth to mention that the BV variational principle has been applied to this model in ref. [74]. The BV gives very good improvement beyond mean-field in the small χ limit where a perturbative treatment is valid but failed to describe the large χ case where symmetry breaking is important.

4.6 Stochastic Mean-Field with pairing correlations

As we have shown in section 2.5, to describe superfluid systems, it is advantageous to break explicitly the symmetry associated to particle number, the $U(1)$ symmetry. Then, the one-body density ρ is replaced by the generalized density \mathcal{R} that evolves at the mean-field level according to Eq. (48). It has been shown recently that the SMF can be generalized to treat superfluid systems also by taking advantage of the $U(1)$ symmetry breaking. Then, an ensemble of initial conditions $\mathcal{R}^{(n)}(t_0)$ followed by TDHFB evolutions [75]:

$$i\hbar \frac{d}{dt} \mathcal{R}^{(n)}(t) = [\mathcal{H}[\mathcal{R}^{(n)}(t)], \mathcal{R}^{(n)}(t)], \quad (94)$$

are considered. The statistical properties of the elements of density matrix $\mathcal{R}_{\alpha\beta}^{(n)}(t_0)$ are specified in terms of statistical properties of the normal $\rho_{\alpha\beta}^{(n)}(t_0)$ and anomalous $\kappa_{\alpha\beta}^{(n)}(t_0)$ density matrices. Elements of the normal and the anomalous density matrices are uncorrelated Gaussian random numbers with the mean values,

$$\overline{\rho_{\alpha\beta}^{(n)}} = \delta_{\alpha\beta} f_\alpha, \quad \overline{\kappa_{\alpha\beta}^{(n)}} = 0, \quad (95)$$

and the second moments defined by,

$$\overline{\delta\rho_{\alpha\beta}^{(n)} \delta\rho_{\alpha'\beta'}^{(n)*}} = \frac{1}{2} \delta_{\alpha\alpha'} \delta_{\beta\beta'} [f_\alpha(1-f_\beta) + f_\beta(1-f_\alpha)], \quad (96)$$

$$\overline{\delta\kappa_{\alpha\beta}^{(n)} \delta\kappa_{\alpha'\beta'}^{(n)*}} = \frac{1}{2} \delta_{\alpha\alpha'} \delta_{\beta\beta'} [f_\alpha f_\beta + (1-f_\alpha)(1-f_\beta)] \quad (97)$$

Note that here α is a label referring to the quasi-particle basis and f_α denotes the initial quasi-particle occupancy.

Such a generalized description is adequate for the description of pairing correlations and allows for the treatment of effect beyond the independent quasi-particle picture. Similarly to the previous case where pairing was neglected, it can be shown in particular that the above statistical properties properly reproduces the initial quantal fluctuations of the mean-values and fluctuations of generalized "one-body" operators written as (see appendix A of ref. [73]):

$$\hat{Q} = \sum_{ij} Q_{ij}^{11} a_i^\dagger a_j + \sum_{ij} \left(Q_{ij}^{20} a_j a_i + Q_{ji}^{20*} a_i^\dagger a_j^\dagger \right). \quad (98)$$

The method has been benchmarked for a system described by a pairing Hamiltonian (picked fence model) [76]

$$H = \sum_{i=1}^K \varepsilon_i \hat{N}_i + \sum_{ij} G_{ij} \hat{S}_i^+ \hat{S}_j^-, \quad (99)$$

where the different operators \hat{N}_i , \hat{S}_i^+ and \hat{S}_i^- are now related respectively to the occupation, pair creation and pair annihilation operators of the level i . As in the LMG model, the TDHFB equation can be written in terms of the quasi-spin operators expectation values:

$$\frac{d}{dt} \begin{pmatrix} S_i^x(t) \\ S_i^y(t) \\ S_i^z(t) \end{pmatrix} = \begin{pmatrix} 0 & -2\tilde{\varepsilon}_i(t) + 2\Delta_i^y & \\ 2\tilde{\varepsilon}_i(t) & 0 & -2\Delta_i^x \\ -2\Delta_i^y & 2\Delta_i^x & 0 \end{pmatrix} \begin{pmatrix} S_i^x(t) \\ S_i^y(t) \\ S_i^z(t) \end{pmatrix} \quad (100)$$

where $S_i^x = (S_i^+ + S_i^-)/2$, $S_i^y = (S_i^+ - S_i^-)/2i$ and $S_i^z = (N_i - \Omega_i)/2$ denote the expectation values of the corresponding operators (see ref. [73] for more details). Connection with the standard TDHFB theory can be made by noting that $S_i^z(t)$ is directly linked to the normal density while $S_i^x(t)$ and $S_i^y(t)$ corresponds to the real and imaginary part of the anomalous density κ .

In the SMF approach built on TDHFB, the three initial quasi-spin become fluctuating quantities. For each initial condition, the TDHFB equation is then solved in time to improve mean-field. The specific case where the system is assumed to be initially in a non-superfluid phase has been considered was used in Ref. [73]. This situation is similar to the one shown in Fig. 4 where the order parameter can for instance be replaced by the pairing gap. The system has initially a vanishing pairing and therefore is at the position located by the arrow in the figure. Since in a pure mean-field description, the system cannot break the symmetry it will stay at the saddle point. It could be indeed shown that, if the initial pairing correlation is zero, the TDHFB equation reduces to the TDHF evolution and that a Slater determinant is stationary. When SMF is used, non-vanishing pairing can occur event-by-event leading to non-trivial dynamics. As an illustration of the SMF with pairing theory predictive power, the quantity $D(t) = 2 \sum_i n_i(t)(1 - n_i(t))$ that measures the fragmentation of the single-particle states around the Fermi energy, is shown in Fig. 7 and compared to the exact evolution starting from a Slater determinant. Note that the

TDHF approach without fluctuations would lead simply to $D(t) = 0$. Similarly to the case presented in previous

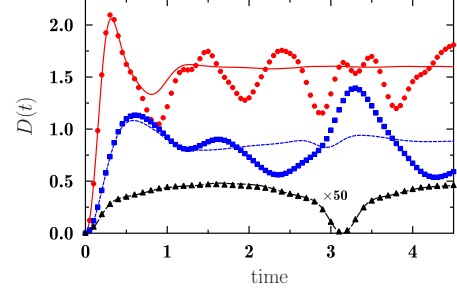


Fig. 7. (color online) Exact evolution of the single-particle fragmentation ($D(t)$) for different pairing interaction strength: weak (black triangles), intermediate (blue squares) and strong (red circles) pairing. The results obtained by averaging over TDHFB trajectories are shown respectively by black long dashed line, blue short dashed line and red solid line (taken from Ref. [75]).

section, the SMF approach is able to provide rather reasonable evolution where TDHF and TDHFB would simply fail.

4.7 A survey of recent applications to nuclear collisions

In recent works, dissipation mechanism [77] and nucleon exchange [78,80] are investigated in the special case of central collisions of heavy-ions near barrier energies. Also, some applications of the SMF approach have been carried out for analyzing early development of spinodal instabilities in nuclear matter [81,82,83,84,85]. In this section, we review recent investigations on dissipative mechanism in central heavy-ion collisions.

4.7.1 Macroscopic reduction of information in mean-field dynamics

For not too heavy systems, in central heavy-ions collisions above the Coulomb barrier lead to fusion, and at below the barrier energies, colliding nuclei exchange a few nucleons and re-separate. Such reactions are often investigated using time-dependent mean-field theories in three dimensions. As an example, Fig. 8 shows the density profiles at the reaction plane, $\rho(x, y, z = 0, t)$ in the $^{40}\text{Ca} + ^{90}\text{Zr}$ collisions at center-of-mass energy $E_{\text{cm}} = 97$ MeV for three different times. The collision energy is below the Coulomb barrier energy and the system re-separate after contact

An important aspect in heavy-ion collisions is the knowledge of transport properties, related to dissipative aspects, during the approaching phase. In particular, the sharing of energy between internal single-particle and collective DOF is essential to understand how the collective phase-space is populated in time. When the system can still be

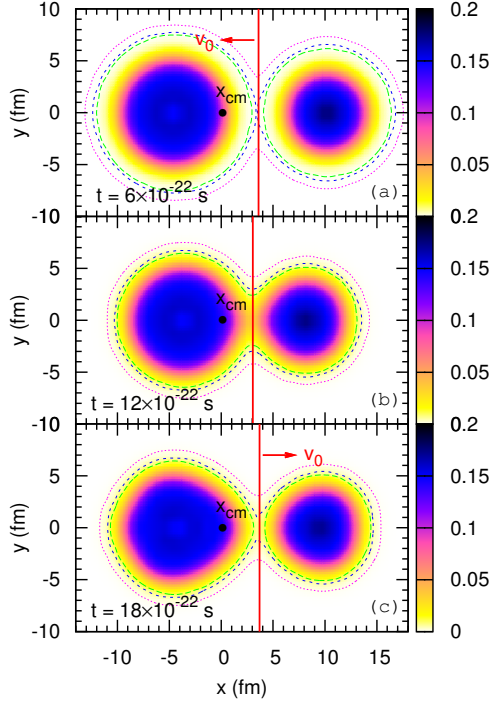


Fig. 8. Nucleon density profiles at the reaction plane, $\rho(x, y, z = 0)$, are indicated by contour plots for the central collision of $^{40}\text{Ca} + ^{90}\text{Zr}$ system at $E_{\text{cm}} = 97$ MeV in units of fm^{-3} . The black dot is the center of mass point. The red lines indicate the positions of the window x_0 and $v_0 = dx_0/dt$ denotes velocity of the window. The three times correspond respectively to before (top), during (middle) and after (bottom) contact (From [80]).

considered as binary, one can get information on dissipation from the microscopic mean-field by focusing on specific macroscopic observables. For instance the evolution of the relative distance gives insight in the energy loss while the number of particles in each nucleus provides direct information on the nucleon exchange process.

A geometric projection method was proposed by introducing the window between projectile-like and target-like nuclei according to the procedure outlined in [7, 77, 78]. Let us assume as a convention that the target is on the right while the projectile is on the left. Any local observable, denoted generically by A of the target or projectile can be computed using

$$A_T(t) = \int d^3\mathbf{r} Q(\mathbf{r}) \Theta(x_0 - x) \rho(\mathbf{r}, \mathbf{r}),$$

$$A_P(t) = \int d^3\mathbf{r} Q(\mathbf{r}) [1 - \Theta(x_0 - x)] \rho(\mathbf{r}, \mathbf{r}), \quad (101)$$

where Θ is the step function. The most common choice for A are either equal to one (for the mass), to the center of mass position, to momentum or to angular momentum. With proper combinations of these quantities, one can construct a set of specific observables, denoted generically by $\{A_\lambda\}$ associated to the relative motion or relative

particle content. At the mean-field level, one can anticipate that the equation of motion will reduce to a set of equations:

$$\frac{d}{dt} A_\lambda(t) = \mathcal{F}(A_\lambda(t)) + \mathcal{V}(A_\lambda(t), t). \quad (102)$$

The two terms respectively stand for a driving force stemming from a potential energy surface in collective space and a dissipative kernel. Note that dissipation of one-body type is automatically contained in TDHF.

It is anticipated that one-body dissipation is rather well described by mean-field. However, fluctuations leading to the dispersion of one-body DOF are strongly underestimated. When initial fluctuations are included in the SMF framework, the macroscopic equation of motion will be approximately transformed as:

$$\frac{d}{dt} A_\lambda^{(n)}(t) = \mathcal{F}(A_\lambda^{(n)}(t)) + \mathcal{V}(A_\lambda^{(n)}(t), t) + \delta\xi_\lambda^{(n)}(t) \quad (103)$$

where a new fluctuating term $\delta\xi_\lambda^{(n)}(t)$ appears. The properties of the fluctuating quantity will depend on the specific collective observables and will in general be rather complex and non-markovian. In the markovian limit, as we will see in examples below, the macroscopic evolution will be similar to a Brownian motion where fluctuations are related to the set of second moment $\delta\xi_\lambda^{(n)}(t) \delta\xi_{\lambda'}^{(n)}(t')$.

4.7.2 Energy dissipation

The powerfulness and applicability of the SMF have been recently illustrated in fusion reactions by extending the work of ref. [7, 79]. Using a macroscopic reduction of the stochastic mean-field evolution, central collisions leading to fusion have been mapped to a one-dimensional macroscopic Langevin evolution on the relative distance R between the two nuclei given by [77]:

$$\dot{P}^{(n)} = -\partial_R U(R^{(n)}) - \gamma[R^{(n)}] \dot{R}^{(n)} + \xi_P^{(n)}(t). \quad (104)$$

$U(R^{(n)})$ and $\gamma(R^{(n)})$ denote the nuclear+coulomb potential and dissipation associated to one-body friction respectively and are already present at the mean-field level [7, 79]. $\xi_P^{(n)}(t)$ is a Gaussian random force acting on the relative motion reflecting stochasticity in the initial value. This fluctuating part leads to diffusion in collective space which can be approximated by

$$\overline{\xi_P^{(n)}(t) \xi_P^{(n)}(t')} \simeq 2\delta(t - t') D_{PP}(R),$$

where $D_{PP}(R)$ denotes the momentum diffusion coefficient. The latter term is nothing but the one that is missing in the original theory and is of primer importance to properly describe observables fluctuations. An example of reduced friction $\beta(R) \equiv \gamma(R)/\mu(R)$ and diffusion coefficients $D_{PP}(R)$ estimated from the macroscopic reduction of SMF is given in Fig. 9 for the head-on $^{40}\text{Ca} + ^{40}\text{Ca}$ collision.

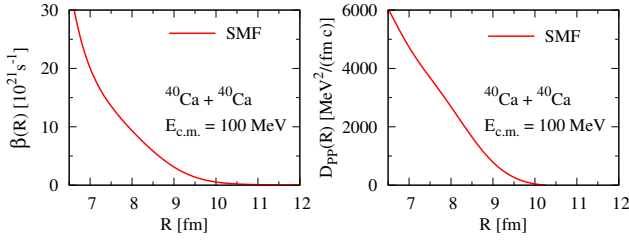


Fig. 9. (Color online) Evolution of reduced friction (left) and diffusion coefficient (right) as a function of the relative distance for the head-on $^{40}\text{Ca} + ^{40}\text{Ca}$ collision at center of mass energy $E_{\text{c.m.}} = 100 \text{ MeV}$.

4.7.3 Nucleon exchange

The possibility to estimate transport coefficients associated to fluctuation and dissipation from a fully microscopic quantum transport theory is a major breakthrough. However, to be really convincing, one should in addition prove that the increase of fluctuations is consistent with experimental observations. To prove that SMF can be a predictive framework, we have recently considered transfer reactions [78]. Fragment mass distributions deduced from Heavy-Ion reactions have been extensively studied. It is seen that the dispersion in mass scales approximately with the average number of exchanged nucleons. While mean-field properly describes the latter, it miserably fails to account for the dispersion. This phenomena is rather well understood in macroscopic models but has not been yet reproduced microscopically. To address this issue, we have considered head-on collisions below the Coulomb barrier. In that case, nuclei approach, exchange some nucleons and then re-separate. Similarly to the relative distance case, a macroscopic reduction onto the projectile (resp. target) mass, denoted by $A_P^{(n)}$ (resp. $A_T^{(n)}$) can be introduced. For small fluctuations, the ensemble average quantities are equivalent to the results obtained by the standard mean-field approximation. As a result, the Langevin equation for the nucleon exchange becomes,

$$\frac{d}{dt} A_T^{(n)}(t) = v_A(t) + \left(\frac{\partial v_A(t)}{\partial A_T} \right) \delta A_T^{(n)}(t) + \xi_A^{(n)}(t) \quad (105)$$

where v_A is the drift coefficient for nucleon exchange. The quantity $\xi_A^{(n)}(t)$ denotes the fluctuating part of the nucleon flux. Similarly to the momentum case, a simplified markovian assumption leads to:

$$\xi_A^{(n)}(t) \xi_A^{(n)}(t') = 2\delta(t - t') D_{AA}(t), \quad (106)$$

where $D_{AA}(t)$ is the diffusion coefficient for nucleon exchange. This result establishes the connection with the nucleon exchange picture developed in the 80's has been made [77, 78]. In particular, computable expressions of the drift and diffusion coefficients were proposed allowing for quantitative description. Fig. 10 illustrates the diffusion coefficients obtained in the central collisions of $^{40}\text{Ca} + ^{90}\text{Zr}$ system as a function of time and at center-of-mass energies below the barrier, $E_{\text{cm}} = 93 \text{ MeV}$ (c) and $E_{\text{cm}} = 97$

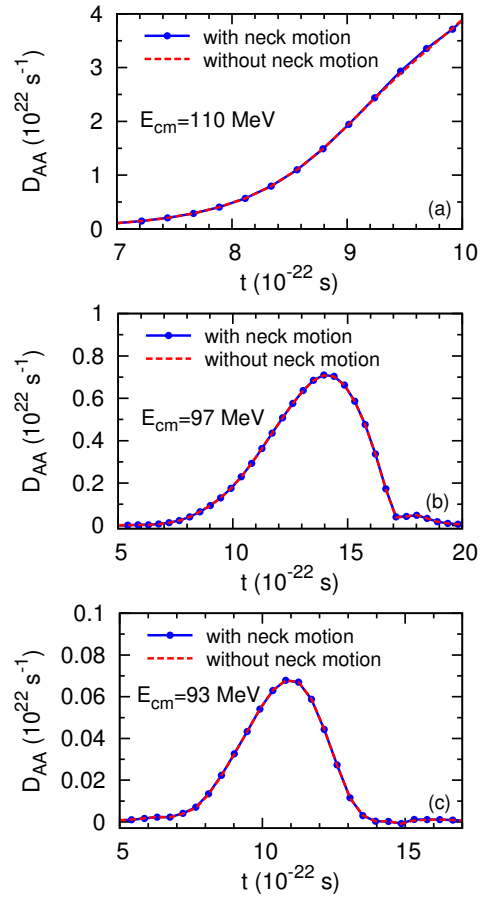


Fig. 10. (color online) Nucleon diffusion coefficients are plotted versus time in central collisions of $^{40}\text{Ca} + ^{90}\text{Zr}$ system at three different center-of-mass energies. (for more details see [80])

MeV (b), and above the barrier energy $E_{\text{cm}} = 110 \text{ MeV}$ (a).

Employing the Langevin Eq. (105) we can calculate the variance $\sigma_{AA}^2(t) = \langle (A_T^\lambda)^2 \rangle - \langle A_T^\lambda \rangle^2$ of fragment mass distribution. It follows that the variance is determined by

$$\frac{d}{dt} \sigma_{AA}^2(t) = 2\alpha(t) \sigma_{AA}^2(t) + 2D_{AA}(t), \quad (107)$$

where $\alpha(t) = \partial v_A(t) / \partial A_T$. Because of very small value of the mean nucleon transfer, we can neglect the contribution from drift term and solve the variance equation (107) to find,

$$\sigma_{AA}^2(t) = 2 \int_0^t D_{AA}(s) ds. \quad (108)$$

An illustration of $\sigma_{AA}^2(t)$ for $^{40}\text{Ca} + ^{40}\text{Ca}$ reactions is given in Fig. 11 and compared to the number of exchanged nucleons, denoted by N_{ex} . In all cases, both quantities are very close from each other and lead to much higher dispersion than the original mean-field. Indeed, with mean-field, the estimated asymptotic values in the latter case are 0.004, 0.008 and 0.008 from low to high energy and

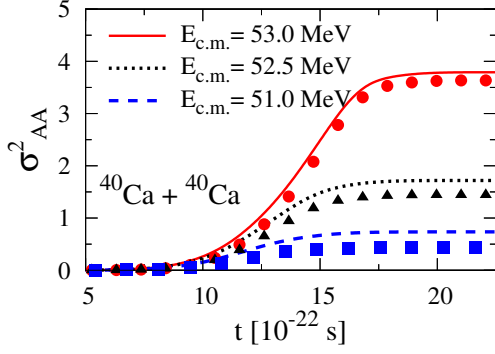


Fig. 11. (Color online) Evolution of σ_{AA}^2 calculated in SMF approach for $^{40}\text{Ca}+^{40}\text{Ca}$ (top) at different center of mass energies. Number of exchanged particles is superimposed by the filled-circles, filled-squares, and filled-triangles from high to low energies. (Adapted from [78])

are much less than the final number of exchanged nucleons that are equal to 0.43, 1.44 and 3.63 respectively. On opposite, the predicted asymptotic mass dispersions are equal to 0.73, 1.72 and 3.79 and is much closer to N_{ex} (see also figure 11). This numerical test provides a strong support for the validity of the stochastic mean-field approach.

From the investigation made on heavy-ion collisions, it has been shown that the SMF theories extend the usual TDHF approach and provide a useful tool to describe not only dissipative aspects but also fluctuations. In particular, it might provide a rather simple approach to overcome most of the shortcomings of TDHF. At present, quantitative aspects have been mainly obtained using a simplified semiclassical approximation. We have observed that, below the Coulomb barrier energies, the semiclassical expression underestimates the nucleon drift deduced from the standard mean-field description with TDHF equations. In the near future, a fully quantal approach avoiding the semi-classical limitations will be required.

4.8 Summary on the SMF theory

The SMF theory has important aspects that make it very attractive (see discussion below). On the theoretical side [62], for small amplitude fluctuations, this model gives a result for the dispersion of a one-body observable that is identical to the one obtained using the Balian-Vénéroni (BV) variational approach [65]. It is also shown that, when the SMF is projected on a collective variable, it gives rise to a generalized Langevin equation [86] that incorporates one-body dissipation and one-body fluctuation mechanisms in accordance with quantal dissipation-fluctuation relation. These connections give a strong support that the SMF approach provides a consistent microscopic description for dynamics of density fluctuations in low energy nuclear reactions.

From the practical point of view, this approach is much simpler than the TDGCM. Indeed, by neglecting the interferences between trajectories, each evolution can be made

independently from the others. In addition, on contrary to the Stochastic TDHF case, that is discussed in section 5.1.1, randomness appears only at the initial time and should not a priori face the difficulty of a statistical explosion of the trajectory number. SMF framework has been recently applied to fusion [77] and transfer reactions [78]. The latter study has in particular pointed out that fluctuations of one-body observables are largely increased as compared to the TDHF and seem consistent with experimental observations. This issue is a long standing problem that was unsolved until now in a fully quantum microscopic approach. Finally recent tests in cases where spontaneous symmetry breaking might be particularly important are very promising.

5 Stochastic Schroedinger equation for N-body problems

In previous section, we have seen that quantum fluctuations beyond mean-field can eventually be incorporated approximately by introducing fluctuations at the initial instant. Here, we are interested in the stochastic treatment of correlations that are not present initially, but that built up in time such as those included in the Extended TDHF or TDDM theories presented in section 3. It is shown below that these correlations can be treated too by adding noise to the self-consistent mean-field, replacing then the initial problem by a set of simpler evolutions of Slater determinants with the great difference, compared to SMF, that the noise is continuously added during the time-evolution.

5.1 Stochastic process in Slater Determinant space

Before describing the specific case of ETDHF, let us understand in a simple manner how a stochastic process can be introduced. Starting from a simple Slater determinant state $|\Psi(t=0)\rangle = |\Phi(t_0)\rangle$, correlations will develop in time and we do expect that the exact Many-Body state writes:

$$|\Psi(t)\rangle = \sum_k c_k(t) |\Phi_k(t)\rangle, \quad (109)$$

where $|\Phi_k\rangle$ denotes a complete (eventually time-dependent) basis of Slater-Determinant states. Accordingly, the many-body density writes

$$D(t) = \sum_{k,k'} c_k(t) c_{k'}^*(t) |\Phi_k(t)\rangle \langle \Phi_{k'}(t)|. \quad (110)$$

The extended and stochastic version of TDHF that will be presented below, implicitly assume that the many-body density can be properly approximated by its diagonal components [87,88]

$$D(t) \simeq \sum_k P_k |\Phi_k(t)\rangle \langle \Phi_k(t)|, \quad (111)$$

where $P_k = |c_k(t)|^2$. The probability P_k obeys a master equation that eventually could be simulated using quantum jumps. The resulting density is obtained through the average over different stochastic paths, i.e.

$$D(t) \simeq \overline{|\Phi_k(t)\rangle \langle \Phi_k(t)|} \quad (112)$$

Physically, this can be understood as follows. The irrelevant degrees of freedom (complex internal degrees of freedom) interacts with the relevant degrees of freedom (single-particle degrees of freedom) and induce a fast decay towards zero for the off-diagonal matrix elements. This phenomenon is known as a decoherence process [89,90].

5.1.1 Extended TDHF in the short memory approximation

The Extended TDHF can eventually be interpreted as an average over quantum jumps between Slater determinants, a theory generally called Stochastic TDHF (STDHF) [87, 91, 92, 88]. Let us first introduce ETDHF using a different technique than the truncation of the BBGKY hierarchy. This theory is expected to be valid in the weak coupling limit, i.e. when the residual interaction introduced in section 2.4.3 is small. Such a theory can indeed be obtained using time-dependent perturbation theory. Starting from an initial density $D(t_0)$, the evolution is given at second order in perturbation theory by

$$i\hbar \frac{dD(t)}{dt} = [H_{\text{MF}}(t), D(t)] - \frac{1}{2\hbar^2} \text{T} \left(\int_{t_0}^t \int_{t_0}^t [V_{\text{res}}(s'), [V_{\text{res}}(s), D(s)]] ds' ds \right),$$

where $\text{T}(\cdot)$ denotes the time-ordering operator and where $V_{\text{res}}(s)$ denotes the residual interaction written in the interaction picture using the mean-field propagator. The expression above is non-local in time, showing that the evolution between a time t and an initial time t_0 depends not only of the system at time t but also on the former time.

The second term in the evolution of $D(t)$ essentially involves two different characteristic times. The first one is the correlation time τ_{cor} , that is defined as

$$\overline{V_{\text{res}}(t) V_{\text{res}}(s)} \propto e^{-|t-s|/\tau_{\text{cor}}}, \quad (113)$$

where the average $\overline{\cdot}$ denotes an average over all possible single-particle states combinations. This time, characteristic of the residual interaction, is directly related to the mean energy Δ exchanged during nucleon-nucleon collisions through the relation $\tau_{\text{cor}} = \hbar/\Delta$ [93]. The second characteristic time, called relaxation time τ_{rel} , corresponds to the time-scale associated to the reorganization of single-particle states.

Here, we consider the limit $\tau_{\text{cor}} \ll \tau_{\text{rel}}$ that is valid for a sufficiently dilute system when the binary collisions are well separated in time and use

$$\overline{V_{\text{res}}(t) V_{\text{res}}(s)} \propto V_{\text{res}}^2(t) F\left(\frac{|t-s|}{\tau_{\text{cor}}}\right). \quad (114)$$

where F is a function that tends to zero over a time-scale τ_{cor} much smaller than the typical time associated to the reorganization of one-body degrees of freedom. In that limit, the density in the integral can be approximated by $D(s) \simeq D(t)$ leading finally to

$$i\hbar \frac{dD(t)}{dt} = [H_{\text{MF}}(t), D(t)] - \frac{g}{2} \left\{ V_{\text{res}}(t) V_{\text{res}}(t) D(t) + D(t) V_{\text{res}}(t) V_{\text{res}}(t) - 2V_{\text{res}}(t) D(t) V_{\text{res}}(t) \right\} \quad (115)$$

where the constant

$$g \equiv \frac{1}{\hbar^2} \iint F(|s-s'|/\tau_{\text{cor}}) ds ds' \quad (116)$$

is introduced. The approximation above leads to an equation of motion for the density $D(t)$ that is local in time, and therefore memory effects have disappeared.

Eq. (115) equation is nothing but a Lindblad equation that is generally found in open quantum systems [94, 95, 34]. Therefore, starting from second-order perturbation theory and assuming the short memory approximation leads naturally to an Open Quantum System equation of motion.

5.1.2 Dissipation in one-body space

Eq. (115) is rather complicated and involves complex many-body operators. Here, we are mainly interested in one-body degrees of freedom. Starting from Eq. (115), the one-body density matrix evolution reads [88]:

$$\frac{d\rho}{dt} = \frac{1}{i\hbar} [h_{\text{MF}}(\rho), \rho] - \frac{g}{2} \mathcal{D}(\rho). \quad (117)$$

$\mathcal{D}(\rho)$, called "dissipator" hereafter, corresponds to the average effect of the residual interaction and reads

$$\langle j | \mathcal{D} | i \rangle = \text{Tr} \left(D \left[[a_i^\dagger a_j, V_{\text{res}}], V_{\text{res}} \right] \right). \quad (118)$$

Assuming that the system is initially in a pure state described by a Slater determinant $|\Phi(t_0)\rangle$ formed of N orthonormal single particle states denoted by $|\alpha\rangle$, the associated initial one-body density matrix reads $\rho = \sum_{\alpha} |\alpha\rangle \langle \alpha|$. Using the residual interaction expression, Eq. (31), $\mathcal{D}(\rho)$ can finally be recast as:

$$\mathcal{D}(\rho) = \text{Tr}_2 [\tilde{v}_{12}, B_{12}], \quad (119)$$

where B_{12} is nothing but the Born term appearing in the Extended TDHF theory. Indeed, a similar expression could have been directly obtained starting from the ETDHF theory in the Markovian limit. Equation (117) is a master equation for the one-body density. It could also be put into a Lindblad form using the fact that the residual interaction can always be decomposed as (see for instance [96, 97])

$$V_{\text{res}} = -\frac{1}{4} \sum_n \lambda_n \mathcal{O}_n^2, \quad (120)$$

where λ_n are real and where the \mathcal{O}_n correspond to a set of commuting Hermitian one-body operators written as $\mathcal{O}_n = \sum_{\bar{\alpha}\alpha} \langle \bar{\alpha} | \mathcal{O}_n | \alpha \rangle a_{\bar{\alpha}}^\dagger a_\alpha$. Reporting in eq. (119), $\mathcal{D}(\rho)$ can be recast as

$$\mathcal{D}(\rho) = \sum_{mn} \Gamma_{mn} [\mathcal{O}_n \mathcal{O}_m \rho + \rho \mathcal{O}_n \mathcal{O}_m - 2\mathcal{O}_m \rho \mathcal{O}_n] \quad (121)$$

The coefficient Γ_{mn} are given by

$$\Gamma_{mn} = \frac{1}{2} \lambda_m \lambda_n \text{Tr}(\mathcal{O}_m (1 - \rho) \mathcal{O}_n \rho). \quad (122)$$

We recognize in this expression, the quantum covariance between the operator \mathcal{O}_n and \mathcal{O}_m , i.e. $\text{Tr}(\mathcal{O}_m (1 - \rho) \mathcal{O}_n \rho) = \langle \mathcal{O}_m \mathcal{O}_n \rangle - \langle \mathcal{O}_m \rangle \langle \mathcal{O}_n \rangle$. Expression (121) has the form of the dissipator appearing usually in the Lindblad equation [34]. Therefore, the evolution of one-body degrees of freedom associated to equation (115) identifies with a Markovian quantum master equation generally obtained in quantum open systems. A large amount of work is devoted to the simulation of such master equation by quantum jump methods (see for instance [98, 99, 100, 101, 34]) and one can take advantage of the most recent advances in this field. This aspect has however rarely been discussed in the context of self-interacting system.

5.1.3 Stochastic process in one-body space

Following ref. [34], we introduce the Hermitian matrix Γ with components Γ_{mn} . An economical method to introduce quantum jumps is to use the unitary transformation u that diagonalizes Γ , i.e. $\Gamma = u^{-1} \gamma u$, where γ is the diagonal matrix of the eigenvalues of Γ . New operators A_k can be defined by the transformation $A_k = \sum_n u_{kn}^{-1} \mathcal{O}_n$. The dissipator is then recast as

$$\mathcal{D}(\rho) = \sum_k \gamma_k [A_k^2 \rho + \rho A_k^2 - 2A_k \rho A_k]. \quad (123)$$

Last expression can be simulated using the average over the stochastic mean-field dynamics:

$$d\rho = \frac{dt}{i\hbar} [h_{MF}(\rho), \rho] - g \frac{dt}{2} \mathcal{D}(\rho) + dB_{sto}, \quad (124)$$

where dB_{sto} is a stochastic one-body operator which, using Ito rules [102] (see also appendix E), reads

$$dB_{sto} = \sum_k \{dW_k (1 - \rho) A_k \rho + dW_k^* \rho A_k (1 - \rho)\} \quad (125)$$

Here dW_k denotes stochastic variables given by $dW_k = -id\xi_k \sqrt{g\gamma_k}$, where $\{d\xi_k\}$ correspond to a set of real gaussian stochastic variables with mean zero and $\overline{d\xi_k d\xi_{k'}} = \delta_{kk'} dt$.

5.1.4 Quantum jump for single-particle states

It is worth noticing that the proposed dissipative equation and its stochastic counterpart are only well defined if the

density is initially prepared as a pure Slater-determinant state. We now turn to the essential properties of equation (124). First, it preserves the number of particles $\text{Tr}(d\rho) = 0$. In addition, if initially $\rho^2 = \rho$, then

$$d\rho d\rho - g \frac{dt}{2} [\rho \mathcal{D}(\rho) + \mathcal{D}(\rho) \rho] = -g \frac{dt}{2} \mathcal{D}(\rho) \quad (126)$$

which is obtained using Ito stochastic rules and retaining only terms linear in dt . Last expression demonstrates that $(\rho + d\rho)^2 = \rho + d\rho$. Thus, ρ remains a projector along the stochastic path. As a consequence, the pure state nature of the many-body density matrix is preserved along the stochastic path, i.e. $D = |\Phi(t)\rangle \langle \Phi(t)|$ where $|\Phi\rangle$ is a normalized Slater determinant at all time. The associated stochastic Schroedinger equation for single-particle states reads

$$d|\alpha\rangle = \left\{ \frac{dt}{i\hbar} h_{MF}(\rho) + \sum_k dW_k (1 - \rho) A_k - g \frac{dt}{2} \sum_k \gamma_k [A_k^2 \rho + \rho A_k \rho A_k - 2A_k \rho A_k] \right\} |\alpha\rangle.$$

This last expression can be directly used for practical applications.

In this section, we have shown that the effect of residual interaction at second order in perturbation and projected on one-body degrees of freedom gives the Extended TDHF approximation in the short-memory time (Markovian) approximation. In such a limit, starting from a pure Slater Determinant state, the dissipative dynamics can be replaced by a quantum jump process where the N-body state remains a SD along each stochastic trajectory. The possibility to account for the effect of correlation on top of a mean-field dynamics has been discussed extensively in the early 80's. For instance, it has been proposed to treat each direct nucleon-nucleon collisions as a random process [92, 103]. Alternatively, following a similar strategy as the one presented in this section and starting from perturbation theory [87, 91], the Fermi golden rule has been used to introduce a Stochastic TDHF theory. The main difficulty is to avoid the explosion of the number of trajectories and therefore find physical criteria to only follow relevant trajectories. The approach presented here makes more transparent the connection of a many-body system where specific degrees of freedom are of interest and the theory of Open Quantum Systems. In addition, the stochastic evolution of single-particle states are directly the equations that should be implemented in practice. It should however be noted that the possible explosion of trajectories is not the only reason that may limit the application of Stochastic TDHF. Indeed, such a theory is well defined if we start from a Hamiltonian but is less clear in the context of density functional theory that most often is not directly linked to the underlying many-body hamiltonian.

5.2 Exact Quantum Monte-Carlo from functional integrals method

Approximations to the N-body problem such as ETDHF, STDHF or SMF focus on one-body degrees of freedom. In these framework some many-body effects such as interferences between different channels are lost. In particular, we do expect that most of the extensions of TDHF presented above will not be able to describe two-body or more complex degrees of freedom. Mean-field theories by projecting out the evolution onto a specific class of degrees of freedom can then be regarded as a system open to the surrounding more complex observables (see for instance discussion in 5.1.1). From the Open Quantum System point of view, the introduction of Extended TDHF and then Stochastic TDHF can be considered as a rather standard way to introduce dissipation using first the Nakajima-Zwanzig approach, second the Markovian approximation and then the stochastic unraveling. Less conventional approaches based on quantum Monte-Carlo can be used to treat exactly the dynamics of a system coupled to an environment [114,106]. A similar exact reformulation also exists in the case of interacting particles using the functional integral method.

Functional integrals techniques have often been used to replace the exact Many-Body problem by an average over different "effective" one-body problem [107,108,109]. In ref. [96], the general strategy to obtain ground state properties of a many-body system using Monte-Carlo methods, the so called Shell-Model Monte-Carlo, is described. Recently, this technique has been combined with mean-field theory to obtain Stochastic TDHF equations which in average lead to the exact evolution [110,97]. The goal of the present section is to demonstrate that one could always treat exactly the problem of interacting particle with density given by Eq. (110) by an appropriate stochastic process between Slater determinants. The exact density will then be obtained by an average

$$D(t) \simeq \overline{|\Phi_k(t)\rangle \langle \Phi'_k(t)|} \quad (127)$$

where states in the left differ from states on the right.

5.2.1 Functional integrals for schematic residual interaction:

We again consider that, at a given time, the Many-Body state is a Slater Determinant $|\Psi(t)\rangle = |\Phi\rangle$. For short time step Δt , we have

$$\begin{aligned} |\Psi(t + \Delta t)\rangle &= \exp\left(\frac{\Delta t}{i\hbar} H\right) |\Phi(t)\rangle \\ &\simeq \left(1 + \frac{\Delta t}{i\hbar} H + O(\Delta t)\right) |\Phi(t)\rangle. \end{aligned} \quad (128)$$

Due to the presence of a two-body interaction in H , the state $|\Psi(t + \Delta t)\rangle$ differs from a Slater Determinant. However, it is proved here that it could be replaced exactly by an average over quantum jumps between SD states.

At any time, the Hamiltonian can be decomposed as a mean-field and a residual part. For simplicity, it is first assumed that

$$V_{\text{res}} = A^2, \quad (129)$$

A being a one-body operators. A Gaussian probability $G(x)$ with mean zero and variance 1 is introduced and the complex number $\Delta\omega \equiv \sqrt{\frac{2\Delta t}{i\hbar}}$ is defined as well as the one-body operator $S(\Delta t, x)$ with

$$S(\Delta t, x) \equiv \frac{\Delta t}{i\hbar} H_{\text{MF}} + x \Delta\omega A. \quad (130)$$

Considering the average value of $S(\Delta t, x)$ and keeping only terms up to Δt , we obtain:

$$\begin{aligned} \int_{-\infty}^{+\infty} e^{S(\Delta t, x)} G(x) dx &= 1 + \frac{\Delta t}{i\hbar} H_{\text{MF}} + \bar{x} \Delta\omega A \\ &\quad + \bar{x}^2 (\Delta\omega)^2 A^2 + O(\Delta t) \\ &= 1 + \frac{\Delta t}{i\hbar} H + O(\Delta t). \end{aligned} \quad (131)$$

By averaging over the different realization of x , we recover the exact propagator over short time step. Note that more general relations could be found using the Hubbard-Stratonovich transformation (see for instance [96]). Using the above relation, we see that

$$\begin{aligned} \exp\left(\frac{\Delta t}{i\hbar} H\right) |\Phi\rangle &= \int_{-\infty}^{+\infty} dx G(x) e^{S(\Delta t, x)} |\Phi(t)\rangle \\ &\equiv \int_{-\infty}^{+\infty} dx G(x) |\Phi_x(t + \Delta t)\rangle \end{aligned} \quad (132)$$

Due to the one-body nature of S , each $|\Phi_x(t + \Delta t)\rangle$ is a Slater determinant. Therefore, we have demonstrated that the evolution of the exact state could be replaced by an ensemble of Slater determinants. The technique could be iterated for each $|\Phi_x(t + \Delta t)\rangle$ to obtain the exact long time dynamics as an average over Slater determinant states. In the continuous time $\Delta t \rightarrow dt$, we will introduce the notation

$$|d\Phi\rangle = \left\{ \frac{dt}{i\hbar} H_{\text{MF}} + x d\omega A \right\} |\Phi\rangle \quad (133)$$

which will be called Stochastic Schroedinger Equation and describe the quantum jump process between Slater determinants. Several comments are in order:

- Since $S(\Delta t, x)$ is not a priori Hermitian, the dynamics does not preserves the orthogonality of the single-particle wave-function. Such a non-orthogonality should properly be treated during the time evolution [97,104].
- Starting from a Many-Body density written as $D(t) = |\Phi\rangle \langle \Phi|$, at an intermediate time, the average density writes

$$D(t) = \overline{|\Phi_1(t)\rangle \langle \Phi_2(t)|}, \quad (134)$$

where $|\Phi_1\rangle$ evolves according to Eq. (133) while $\langle\Phi_2|$ evolves according to

$$\langle\Phi_2(t + \Delta t)| = \langle\Phi_2(t)| \exp \left\{ -\frac{\Delta t}{i\hbar} H_{\text{MF}} + y \Delta \omega^* A \right\}.$$

y is a noise independent of x , with mean zero and $\overline{yy} = 1$. Since the evolution is exact, any one-, two- or k -body observable Q estimated through $\langle Q \rangle \equiv \text{Tr}(D(t)Q)$ will follow the exact dynamics [104].

5.2.2 General Many-Body Hamiltonian:

The functional integral method has been introduced above using a schematic separable residual interaction. For a general two-body Hamiltonian, one can take advantage of the decomposition of the residual interaction according to Eq. (120). Therefore, for realistic interactions one should introduce as many stochastic Gaussian independent variables as the number of operators entering in the sum. In practice, this number defines the numerical effort which in general is very large. For this reasons only few applications to the dynamics of rather simple systems exist so far. Last, the extension of above stochastic theories to HFB state has been given in ref. [105].

5.3 Quantum Monte-Carlo method for closed systems from optimal observables evolution

Using the functional integral method, it has been shown above that the exact evolution of particles interacting through a two-body Hamiltonian can be replaced by a set of stochastic evolutions of densities written as $D = |\Phi_a\rangle\langle\Phi_b|$ where both $|\Phi_a\rangle$ and $|\Phi_b\rangle$ are independent particle states. More generally, several studies [110, 97, 111, 112, 113, 114] have shown that the exact dynamics of a many-body system can be replaced by the average over "densities" of the form

$$D(t) = |Q_a\rangle\langle Q_b|, \quad (135)$$

where $|Q_a\rangle$ and $|Q_b\rangle$ belong to a specific class of trial states introduced in section 2.2. One of the disadvantage of the functional integral approach is that the link with observable evolution is highly non-trivial. Here, a different strategy proposed in ref. [115] is introduced to design the quantum Monte-Carlo process. The method is not specifically dedicated to the N -body problem. Therefore, it is presented starting from any class of trial states. The basic idea is to directly use observables evolution to deduce the stochastic contribution. In section 2.2, it is shown that mean-field approximation can be regarded as the optimal path for the expectation values of the observables $\{\langle A_\alpha \rangle\}$ that generate transformations between trial states. Accordingly, mean-field dynamic insures that the exact Ehrenfest evolution is obtained for these observables over short time. Here, we consider evolution within

the class of trial states given by

$$|Q_a + \delta Q_a\rangle = e^{\sum_\alpha \delta q_\alpha^{[a]} A_\alpha} |Q_a\rangle, \quad (136)$$

$$|Q_b + \delta Q_b\rangle = e^{\sum_\alpha \delta q_\alpha^{[b]} A_\alpha} |Q_b\rangle, \quad (137)$$

where now $\delta q_\alpha^{[a]}$ and $\delta q_\alpha^{[b]}$ may also contain a fluctuating part.

The aim of the present section is to show that, given a class of trial states, a hierarchy of Monte-Carlo formulations can be systematically obtained, written as

$$\begin{cases} \delta q_\alpha^{[a]} = \delta q_\alpha^a + \delta \xi_\alpha^{[2]} + \delta \xi_\alpha^{[3]} + \dots \\ \delta q_\alpha^{[b]*} = \delta q_\alpha^{b*} + \delta \eta_\alpha^{[2]} + \delta \eta_\alpha^{[3]} + \dots \end{cases} \quad (138)$$

where the second, third... terms represent stochastic variables added on top of the self-consistent evolution. These random terms are optimized to not only insure that the average evolution of $\langle A_\alpha \rangle$ matches the exact evolution at each time step but also that the average evolutions of higher moments $\langle A_\alpha A_\beta \rangle$, $\langle A_\alpha A_\beta A_\gamma \rangle$,... follow the exact Ehrenfest dynamics.

5.3.1 Link between stochastic process and observables evolution

Step 1: deterministic evolution

Assuming first that stochastic contributions $\xi_\alpha^{[i]}$ and $\eta_\alpha^{[i]}$ are neglected in eq. (138), we show how variational principles described previously can be used for mixed densities given by eq. (135). It is worth noticing that variational principles have also been proposed to estimate transition amplitudes [25] (see also discussion in [65]). In that case, different states are used in the left and right hand side of the action. This situation is similar to the case we are considering. We are interested here in the short time evolution of the system, therefore we disregard the time integral in equation (3) and consider directly the action

$$S = \text{Tr} (\{ i\hbar \partial_t^\triangleright - i\hbar \partial_t^\triangleleft - H \} D). \quad (139)$$

Starting from the above action, different aspects discussed in section 2.1 can be generalized to the case of densities formed of trial states couples. For instance, the minimization with respect to the variations $\langle \delta Q_b |$ and $|\delta Q_a\rangle$ leads to the two conditions

$$\begin{cases} i\hbar \langle Q_b | A_\alpha | dQ_a \rangle = \langle Q_b | A_\alpha H | Q_a \rangle, \\ i\hbar \langle dQ_b | A_\alpha | Q_a \rangle = \langle Q_b | H A_\alpha | Q_a \rangle, \end{cases} \quad (140)$$

from which we deduce that

$$i\hbar \frac{d}{dt} \langle A_\alpha \rangle = \langle [A_\alpha, H] \rangle, \quad (141)$$

where $\langle A_\alpha \rangle = \langle Q_b | A_\alpha | Q_a \rangle$. Therefore, the minimization of the action again insures that the exact Ehrenfest evolution is followed by the A_α observable over one time step.

Similarly, the evolution of both $|Q_a\rangle$ and $|Q_b\rangle$ are given by ³

$$\begin{cases} |dQ_a\rangle = \sum_{\alpha} dq_{\alpha}^a A_{\alpha} |Q_a\rangle = \frac{dt}{i\hbar} \mathcal{P}_1 H |Q_a\rangle \\ \langle dQ_b| = \langle Q_b| \sum_{\alpha} dq_{\alpha}^{b*} A_{\alpha} = -\frac{dt}{i\hbar} \langle Q_b| H \mathcal{P}_1 \end{cases}$$

where \mathcal{P}_1 now reads

$$\mathcal{P}_1 = \sum_{\alpha\beta} A_{\alpha} |Q_a\rangle C_{\alpha\beta}^{-1} \langle Q_b| A_{\beta}. \quad (142)$$

In opposite to previous section, \mathcal{P}_1 cannot be interpreted as a projector onto the space of observable. Indeed, $C_{\alpha\beta} = \langle Q_b | A_{\alpha} A_{\beta} | Q_a \rangle$ is not anymore a metric for that space. However, the total Hamiltonian can still be split into two parts

$$H = \mathcal{P}_1 H + (1 - \mathcal{P}_1) H = H \mathcal{P}_1 + H(1 - \mathcal{P}_1) \quad (143)$$

the first part being responsible for the mean-field deterministic evolution.

Step 2 : Introduction of Gaussian stochastic processes:

In this section, it is shown that the description of the dynamics can be further improved by introducing diffusion in the Hilbert space of trial states. We consider that the evolutions of $q_{\alpha}^{[a]}$ and $q_{\alpha}^{[b]}$ now read

$$\begin{aligned} dq_{\alpha}^{[a]} &= dq_{\alpha}^a + d\xi_{\alpha}^{[2]}, \\ dq_{\alpha}^{[b]*} &= dq_{\alpha}^{b*} + d\eta_{\alpha}^{[2]}, \end{aligned}$$

where $d\xi_{\alpha}^{[2]}$ and $d\eta_{\alpha}^{[2]}$ correspond to two sets of stochastic gaussian variables with mean values equal to zero and variances verifying

$$d\xi_{\alpha}^{[2]} d\xi_{\beta}^{[2]} = d\omega_{\alpha\beta}, \quad d\eta_{\alpha}^{[2]} d\eta_{\beta}^{[2]} = d\sigma_{\alpha\beta}, \quad d\xi_{\alpha}^{[2]} d\eta_{\beta}^{[2]} = 0$$

We assume that $d\omega_{\alpha\beta}$ and $d\sigma_{\alpha\beta}$ are proportional to dt . The advantage of introducing the Monte-Carlo method can be seen in the average evolutions of the states. Keeping only linear terms in dt in eq. (137) gives for instance

$$\begin{aligned} \overline{|dQ_a\rangle} &= \left\{ \sum_{\alpha} dq_{\alpha}^a A_{\alpha} \right. \\ &\quad \left. + \sum_{\alpha<\beta} d\omega_{\alpha\beta} (A_{\alpha} A_{\beta} + A_{\beta} A_{\alpha}) \right\} |Q_a\rangle \quad (144) \end{aligned}$$

Mean field approximation leads to an approximate treatment of the dynamics associated to effective Hamiltonian which can only be written as a linear superposition of the A_{α} (see Eq. (189)). Last expression underlines that, while the states remain in a simple class of trial states, the average evolution can now simulate the evolution with an effective Hamiltonian containing not only linear but also quadratic terms in A_{α} .

The goal is now to take advantage of this generalization and reduce further the distance between the average evolution and the exact one. The most natural generalization of mean-field is to minimize the average action

$$S = \overline{\text{Tr}(\{i\hbar\partial_t^{\dagger} - i\hbar\partial_t - H\} D)}, \quad (145)$$

with respect to the variations of different parameters, i.e. δq_{α}^a , δq_{α}^{b*} , $\delta\omega_{\alpha\beta}$ and $\delta\sigma_{\alpha\beta}$. In the following, a formal solution of the minimization procedure is obtained. The variational principle applied to stochastic process generalizes the deterministic case by imposing that not only that expectation values $\langle A_{\alpha} \rangle$ but also the second moments $\langle A_{\alpha} A_{\beta} \rangle$, follow the Ehrenfest theorem prescription.

Effective Hamiltonian dynamics deduced from the minimization:

The variations with respect to δq_{α}^{b*} and $\delta\sigma_{\alpha\beta}$ give two sets of coupled equations between dq_{α}^a and $d\omega_{\alpha\beta}$. The formal solution of the minimization can however be obtained by making an appropriate change on the variational parameters prior to the minimization. In the following, the notation $B_{\nu} = A_{\alpha} A_{\beta} + A_{\beta} A_{\alpha}$ is introduced where ν denotes (α, β) with $\alpha < \beta$. Starting from the general form of the effective evolution (144), we dissociate the part which contributes to the evolution of the $\langle A_{\alpha} \rangle$ from the rest. This could be done by introducing the projection operator \mathcal{P}_1 . Equation (144) then reads

$$\overline{|dQ_a\rangle} = \left\{ \sum_{\alpha} dz_{\alpha}^a A_{\alpha} + \sum_{\nu} d\omega_{\nu} (1 - \mathcal{P}_1) B_{\nu} \right\} |Q_a\rangle \quad (146)$$

where the new set of parameters dz_{α}^a are given by

$$dz_{\alpha}^a = dq_{\alpha}^a + \sum_{\beta\nu} d\omega_{\nu} C_{\alpha\beta}^{-1} \langle Q_b | A_{\beta} B_{\nu} | Q_a \rangle. \quad (147)$$

Similarly, the average evolution $\langle dQ_b|$ transforms into

$$\overline{\langle dQ_b|} = \langle Q_b| \left\{ \sum_{\alpha} dz_{\alpha}^{b*} A_{\alpha} + \sum_{\nu} d\sigma_{\nu} B_{\nu} (1 - \mathcal{P}_1) \right\} \quad (148)$$

where dz_{α}^{b*} is given by

$$dz_{\alpha}^{b*} = dq_{\alpha}^{b*} + \sum_{\beta\nu} d\sigma_{\nu} \langle Q_b | B_{\nu} A_{\beta} | Q_a \rangle C_{\beta\alpha}^{-1}. \quad (149)$$

In the following, we write $B'_{\nu} = (1 - \mathcal{P}_1) B_{\nu}$ and $B''_{\nu} = B_{\nu} (1 - \mathcal{P}_1)$. The great interest of this transformation is to have $\langle A_{\alpha} B'_{\nu} \rangle = 0$ and $\langle B''_{\nu} A_{\alpha} \rangle = 0$ for all α and ν . Accordingly, the variations with respect to δz_{α}^{b*} and δz_{α}^a lead to

$$\begin{cases} i\hbar \overline{\langle Q_b | A_{\alpha} | dQ_a \rangle} = \langle Q_b | A_{\alpha} H | Q_a \rangle \\ i\hbar \overline{\langle dQ_b | A_{\alpha} | Q_a \rangle} = \langle Q_b | H A_{\alpha} | Q_a \rangle, \end{cases} \quad (150)$$

leading to closed equations for the variations dz_{α}^a and dz_{α}^{b*} that are decoupled from the evolution of $d\omega_{\nu}$ and $d\sigma_{\nu}$.

³ For simplicity, we consider here non-necessarily normalized states.

These equations are identical to the ones derived in step 1 and can be again inverted as

$$\sum_{\alpha} dz_{\alpha}^a A_{\alpha} |Q_a\rangle = \frac{dt}{i\hbar} \mathcal{P}_1 H |Q_a\rangle, \quad (151)$$

$$\langle Q_b | \sum_{\alpha} dz_{\alpha}^{b*} A_{\alpha} = -\frac{dt}{i\hbar} \langle Q_b | H \mathcal{P}_1. \quad (152)$$

On the other hand, the variations with respect to $\delta\sigma_{\nu}$ and $\delta\omega_{\nu}$ lead to

$$\begin{cases} i\hbar \overline{\langle Q_b | B_{\nu}'' | dQ_a \rangle} = \langle Q_b | B_{\nu}'' H | Q_a \rangle, \\ i\hbar \overline{\langle dQ_b | B_{\nu}' | Q_a \rangle} = \langle Q_b | H B_{\nu}' | Q_a \rangle, \end{cases} \quad (153)$$

which again gives closed equations for $d\omega_{\nu}$ and $d\sigma_{\nu}$. These equations can be formally integrated by introducing the two projectors \mathcal{P}_2 and \mathcal{P}_2' associated respectively to the subspaces of operators $B_{\nu}(1 - \mathcal{P}_1)$ and $(1 - \mathcal{P}_1)B_{\nu}$. \mathcal{P}_2 differs from \mathcal{P}_2' due to the fact that B_{ν} operators and A_{α} operators do not a priori commute. Then, the effective evolution given by eq. (144) becomes

$$\begin{aligned} \overline{|dQ_a\rangle} &= \frac{dt}{i\hbar} \left(\sum_{\alpha} dz_{\alpha}^a A_{\alpha} + (1 - \mathcal{P}_1) \sum_{\nu} d\omega_{\nu} B_{\nu} \right) |Q_a\rangle \\ &= \frac{dt}{i\hbar} (\mathcal{P}_1 + \mathcal{P}_2) H |Q_a\rangle, \end{aligned} \quad (154)$$

while

$$\overline{\langle dQ_b |} = -\frac{dt}{i\hbar} \langle Q_b | H (\mathcal{P}_1 + \mathcal{P}_2'). \quad (155)$$

In both cases, the first part corresponds to the projection of the exact dynamics on the space of observable $\langle A_{\alpha} \rangle$. The second term corresponds to the projection on the subspace of the observable $\langle A_{\alpha} A_{\beta} \rangle$ "orthogonal" to the space of the $\langle A_{\alpha} \rangle$.

Interpretation in terms of observable evolution:

The variation with respect to an enlarged set of parameters does a priori completely determine the deterministic and stochastic evolution of the two trial state vectors. The associated average Schroedinger evolution corresponds to a projected dynamics. The interpretation of the solution obtained by variational principle is rather clear in terms of observable evolution. Indeed, from the two variational conditions, we can easily deduce that

$$\begin{aligned} \overline{d\langle A_{\alpha} \rangle} &= \langle [A_{\alpha}, H] \rangle, \\ \overline{d\langle B_{\nu} \rangle} &= \frac{dt}{i\hbar} \langle [B_{\nu}, H] \rangle. \end{aligned}$$

In summary, using the additional parameters associated with the stochastic contribution as variational parameters for the average action given by eq. (145), one can further reduce the distance between the simulated evolution and the exact solution. When gaussian noises are used, this is equivalent to impose that the evolution of the correlations between operators A_{α} obtained by averaging over different stochastic trajectories also matches the exact evolution.

Step 3: Generalization

If the Hamiltonian H applied to the trial state can be written as a quadratic Hamiltonian in terms of A_{α} and if the trial states form an over-complete basis of the total Hilbert space, then the above procedure provides an exact stochastic reformulation of the problem. If it is not the case, the above methods can be generalized by introducing higher order stochastic variables. Considering now the more general form

$$\begin{cases} \delta q_{\alpha}^{[a]} = \delta q_{\alpha}^a + \delta \xi_{\alpha}^{[2]} + \delta \xi_{\alpha}^{[3]} + \dots \\ \delta q_{\alpha}^{[b]*} = \delta q_{\alpha}^{b*} + \delta \eta_{\alpha}^{[2]} + \delta \eta_{\alpha}^{[3]} + \dots \end{cases}$$

we suppose now that the only non vanishing moments for $d\xi_{\alpha}^{[k]}$ and $d\eta_{\alpha}^{[k]}$ are the moments of order k (which are then assumed to be proportional to dt). For instance, we assume that $d\xi_{\alpha}^{[3]}$ verifies

$$\overline{d\xi_{\alpha}^{[3]}} = \overline{d\xi_{\alpha}^{[3]} d\xi_{\beta}^{[3]}} = 0, \quad (156)$$

$$\overline{d\xi_{\alpha}^{[3]} d\xi_{\beta}^{[3]} d\xi_{\gamma}^{[3]}} \neq 0. \quad (157)$$

Then without going into details, the method presented in step 2 can be generalized. The average evolutions of the trial states will be given by

$$\begin{aligned} \overline{|dQ_a\rangle} &= \frac{dt}{i\hbar} \{ \mathcal{P}_1 + \mathcal{P}_2 + \mathcal{P}_3 + \dots \} H |Q_a\rangle \\ \overline{\langle dQ_b |} &= -\frac{dt}{i\hbar} \langle Q_b | H \{ \mathcal{P}_1 + \mathcal{P}_2' + \mathcal{P}_3' + \dots \} \end{aligned}$$

where the first terms contain all the information on the evolution of the $\langle A_{\alpha} \rangle$, the second terms contain all the information on the evolution of the $\langle A_{\alpha} A_{\beta} \rangle$ which is not accounted for by the first term, the third terms contain all the information on the evolution of the $\langle A_{\alpha} A_{\beta} A_{\gamma} \rangle$ which is not contained in the first two terms, ... The procedure described here gives an exact Monte-Carlo formulation of a given problem if the Hamiltonian H applied on $|Q_a\rangle$ or $\langle Q_b |$ can be written as a polynomial of A_{α} . If the polynomial is of order k , then the sum stops at \mathcal{P}_k .

5.3.2 Summary and discussion on applications

Considering a restricted class of trial state vectors associated to a set of observable A_{α} , a hierarchy of stochastic approximations can be obtained. The method discussed here insures that at the level k of the hierarchy, all moments of order k or below of the observable A_{α} evolve according to the exact Ehrenfest equation over short time. The Monte-Carlo formulation might becomes exact if the Hamiltonian applied to the trial state writes as a polynomial of the A_{α} operators.

Aside of the use of variational techniques, we end up with the following important conclusion: *Given an initial density $D = |Q_a\rangle \langle Q_b|$ where both states belongs to a given class of trial states associated to a set of operators A_{α} , we can always find a Monte-Carlo process which preserves*

the specific form of D and insures that expectations values of all moments of the A_α up to a certain order k evolve in average according to the Ehrenfest theorem associated to the exact Hamiltonian at each time step and along each trajectory.

This statement is referred to as the "existence theorem" in ref. [115]. Such a general statement is very useful in practice to obtain stochastic processes. Indeed, the use of variational techniques might become rather complicated due to the large number of degrees of freedom involved. An alternative method is to take advantage of the natural link made between the average effective evolution deduced from the stochastic evolution and the phase-space dynamics. Indeed, according to the existence theorem, we know that at a given level k of approximation, the dynamics of each trial state can be simulated by an average effective Hamiltonian insuring that all moments of order k or below matches the exact evolution. In practice, it is easier to express the exact evolution of the moments and then "guess" the associated stochastic process. Many examples taken from general quantum mechanics, atomic physics, interacting bosons or fermions have been given in ref. [115].

As an illustration, let us come back to the problem of interacting fermions with a two-body Hamiltonian. Assuming that at a given time step, the exact density can be recovered by averaging over an ensemble of densities

$$D = |\Phi_a\rangle \langle \Phi_b|, \quad (158)$$

where both states correspond to SD states. If we denote by $\{|\beta_i\rangle\}_{i=1,N}$ and $\{|\alpha_i\rangle\}_{i=1,N}$ the set of N single-particle states, we assume in addition that for each couples of SD, associated singles-particle wave-functions verify $\langle \beta_j | \alpha_i \rangle = \delta_{ij}$. Accordingly, the one-body density matrix associated to a given D reads [116, 104, 88]

$$\rho_1 = \sum_i |\alpha_i\rangle \langle \beta_i|. \quad (159)$$

It can be easily verified that $\rho_1^2 = \rho_1$ and $\text{Tr}(D) = 1$. For each D given by eq. (158), the two-body density writes as $\rho_{12} = (1 - P_{12})\rho_1\rho_2$. The evolution of ρ_1 and ρ_{12} over one time step are given by the two first equations of the BBGKY hierarchy which reads in that case

$$i\hbar \frac{d}{dt} \rho_1 = [h_{MF}, \rho_1], \quad (160)$$

$$\begin{aligned} i\hbar \frac{d}{dt} \rho_{12} = & [h_{MF}(1) + h_{MF}(2), \rho_{12}] \\ & + (1 - \rho_1)(1 - \rho_2)v_{12}\rho_1\rho_2 \\ & - \rho_1\rho_2v_{12}(1 - \rho_1)(1 - \rho_2). \end{aligned} \quad (161)$$

Again, decomposing the interaction as a sum over separable terms built from a complete set of hermitian operators O_n (Eq. (120)), the previous expression can be simulated by a stochastic dynamics in phase-space given by

$$\begin{aligned} d\rho_1 = & \frac{dt}{i\hbar} [h_{MF}, \rho_1] + \sum_n d\xi_n^{[2]} (1 - \rho_1) O_n \rho_1 \\ & + \sum_n d\eta_n^{[2]} \rho_1 O_n (1 - \rho_1), \end{aligned} \quad (162)$$

where $d\xi_\lambda^{[2]}$ and $d\eta_\lambda^{[2]}$ are two sets of independent stochastic variables with mean zero and verifying $d\xi_n^{[2]} d\xi_{n'}^{[2]} = \delta_{nn'} \frac{dt}{i\hbar} \lambda_n$ and $d\eta_n^{[2]} d\eta_{n'}^{[2]} = -\delta_{nn'} \frac{dt}{i\hbar} \lambda_n$. This stochastic master equation is exact and can equivalently be replaced by a Stochastic Schrödinger equation for single-particle wave-functions given by

$$\begin{aligned} d|\alpha_i\rangle &= \left(\frac{dt}{i\hbar} h_{MF} + \sum_n d\xi_n^{[2]} (1 - \rho_1) O_n \right) |\alpha_i\rangle, \\ d\langle \beta_i| &= \langle \beta_i| \left(-\frac{dt}{i\hbar} h_{MF} + \sum_n d\eta_n^{[2]} O_n (1 - \rho_1) \right). \end{aligned}$$

This stochastic equation preserves the property $\langle \beta_j | \alpha_i \rangle = \delta_{ij}$. Therefore, it corresponds in many-body space to a Monte-Carlo procedure which transforms the initial set of densities into another set of densities with identical properties.

Using the present method, quantum Monte-Carlo approach to a closed system can be rather easily guessed. Application of QMC remains very challenging. First, in most physical cases, statistical fluctuations around the mean trajectory become very large for long time evolutions. As a consequence, the number of trajectories necessary to properly describe the problem increases very fast and prevent from using such a technique. Specific methods, that explicitly use the QMC flexibility, can however be proposed to reduce statistical fluctuations [104]. Second, implementation of QMC requires to solve non-linear stochastic equations. It turns out that trajectories can make large excursion in unphysical regions of the phase-space leading to unstable trajectories (also called spikes). This is a problem which seems to be recurrent in the context of quantum stochastic mechanics both with Stochastic Schrödinger Equation [110] or stochastic evolution in phase-space [117]. Therefore, to take full advantage of these techniques one should develop specific numerical methods. This has been done for instance in refs. [110, 118, 119] using the fact that stochastic equations are generally not unique.

6 Summary

In this review, we have summarized some of the possible ways to extend TDHF, some of them are able to incorporate pairing correlations (like TDHFB or TDDM) whereas others concentrates on direct nucleon-nucleon collisions (ETDHF, STDHF) or initial correlation effects (SMF). Table 1 gives an overview of the theory introduced here while figure 3 illustrates the differences between the three stochastic methods, namely Stochastic TDHF, SMF and QMC. While very promising applications of these theories to the nuclear many-body problem remain very challenging and some of the above theories have never been used. A first difficulty is the computational effort required to treat time dependent methods beyond mean-field. However, besides numerical difficulties, more fundamental problems persist. Indeed, a second critical aspects which has not

been discussed here is that all applications of dynamical quantum transport theories to nuclear reactions are nowadays possible thanks to the introduction of effective interactions (essentially Skyrme like). These interactions have led to the more general concept of Energy Density Functional (EDF) and are expected, in a similar way as Density Functional Theory (DFT) in condensed matter, to incorporate most of the correlations already at the mean-field level. Then, the very notion of "mean-field" and/or "beyond mean-field" framework becomes ill defined. All theories presented in this chapter (extended, stochastic...) start from a Many-Body Hamiltonian. In the EDF context, such an Hamiltonian, although it exists, is not simply connected to the EDF itself. As a consequence, the Hamiltonian derivation could only serve as a guideline and a proper formulation in the EDF framework is mandatory. Large debates exist nowadays on the validity and foundation of the nuclear EDF applied to static properties of nuclei.

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A Density matrices

In this appendix, some relationship and definition related to densities in many-body systems and that are useful in this article, are summarized. Given a many-body state $|\Psi\rangle$. We define the k-body density as

$$\langle k' \dots 1' | \rho_{1, \dots, k} | 1 \dots k \rangle = \langle \Psi | a_1^+ \dots a_k^+ a_{1'} \dots a_{k'} | \Psi \rangle \quad (163)$$

This is equivalent to define the 1, 2, 3-body density as (note the $1/k!$ factor compared to [116])

$$\begin{aligned} \rho_1(x_1 | x'_1) &= A \int \Psi(x_1, \dots, x_A) \Psi^*(x_1, \dots, x_A) d(2 \dots A), \\ \rho_{12}(x_1, x_2 | x'_1, x'_2) &= A(A-1) \\ &\times \int \Psi(x_1, x_2, \dots, x_A) \Psi^*(x_1, x'_1, \dots, x_A) d(3 \dots A), \\ &\dots \end{aligned}$$

Here A is the number of particles and the notation

$$d(k \dots A) = dx_k \dots dx_A dx'_k \dots dx'_A, \quad (164)$$

is used. With this relations, densities are normalized as

$$Tr(\rho_{1, \dots, k}) = \frac{A!}{(A-k)!}, \quad (165)$$

and verifies the recurrence relation

$$\rho_{1 \dots k} = \frac{1}{A-k} Tr_{k+1} \rho_{1, \dots, k+1}. \quad (166)$$

A.1 Two and three-body Correlations

C_{12} denotes the two-body correlation matrix and is defined from

$$C_{12} = \rho_{12} - \rho_1 \rho_2 (1 - P_{12}) \quad (167)$$

where P_{12} is the permutation operator ($P_{12}|i j\rangle = |j i\rangle$). Properties of C_{12} are essentially those of ρ_{12} :

– **Hermiticity:**

$$\langle \mathbf{x}_1, \mathbf{x}_2 | C_{12} | \mathbf{x}'_1, \mathbf{x}'_2 \rangle = \langle \mathbf{x}'_1, \mathbf{x}'_2 | C_{12} | \mathbf{x}_1, \mathbf{x}_2 \rangle^* \quad (168)$$

– **Anti-symmetry:**

$$\langle \mathbf{x}_1, \mathbf{x}_2 | C_{12} | \mathbf{x}'_1, \mathbf{x}'_2 \rangle = - \langle \mathbf{x}_1, \mathbf{x}_2 | C_{12} | \mathbf{x}'_2, \mathbf{x}'_1 \rangle \quad (169)$$

– **Consistency between the two and one-body density:** due to the fact that the one-body density can be obtained from the two-body density, C_{12} should fulfill some relations. We have (using $Tr(\rho_1) = N$)

$$Tr_2 \rho_{12} = Tr_2 C_{12} + N \rho_1 - \rho_1^2, \quad (170)$$

since we should also have

$$Tr_2 \rho_{12} = (N-1) \rho_1, \quad (171)$$

we finally deduce the consistency relation

$$Tr_2 C_{12} = -\rho_1(1 - \rho_1). \quad (172)$$

The three-body correlation is defined as

$$\begin{aligned} C_{123} &= \rho_{123} - \rho_1 \rho_2 \rho_3 (1 - P_{12})(1 - P_{13} - P_{23}) \\ &\quad - \rho_1 C_{23} (1 - P_{12} - P_{13}) \\ &\quad - \rho_2 C_{13} (1 - P_{21} - P_{23}) \\ &\quad - \rho_3 C_{12} (1 - P_{31} - P_{32}) \end{aligned}$$

Similarly to the two-body case, the three-body correlation matrix verifies a large number of properties associated to anti-symmetry, particle number conservation...

B Correlations between observables and Projection techniques

To properly introduce the projection onto a subspace of observables, the notion of independence and correlation between observables should be first discussed. The strategy followed here is essentially the same as in the Principal Component Analysis (PCA) used in statistical analysis. Let us consider a set of operators $\{A_\alpha\}$ and a density D describing the properties of a system at a given time which is interpreted as a probability. The $\{A_\alpha\}$ form a subset of the total space of observables. In the following, It is shown how any other observables can be projected out on this subset. Part of the method presented here has been used to introduce stochastic mean-field approaches in closed system in ref. [115]. Readers that are not interest in technical details may skip this part and directly jump

to appendix C.

Creation of an independent set of operators in the $\{A_\alpha\}$ subspace: Observables $\{A_\alpha\}$ are not necessarily statistically independent from each others with respect to the state D . In the following, we will just say that they are D -correlated or D -independent in the opposite case. To measure correlation between observables, we introduce the variance-covariance matrix defined as ⁴:

$$C_{\alpha\beta} = \langle A_\alpha A_\beta \rangle - \langle A_\alpha \rangle \langle A_\beta \rangle, \quad (174)$$

has non zero off-diagonal matrix elements. We assume here that the $\{A_\alpha\}$ are hermitian operators implying that C is also hermitian. Below, the different notations:

$$C_{\alpha\beta} = C(A_\alpha, A_\beta) = \langle \langle A_\alpha | A_\beta \rangle \rangle \quad (175)$$

will be used. In the following, it is assumed that C is not singular. Note that, if it is the case, it does only mean that there is redundant information and that the subset of observables can be further reduced. C could be diagonalized by a unitary transformation U and has only positive eigenvalues denoted by λ_α ⁵. It is then convenient to introduce a new set of operators $\{e_\alpha^\dagger\}$, defined from the relationship

$$e_\alpha = \frac{1}{\sqrt{\lambda_\alpha}} \sum_\beta U_{\alpha\beta}^{-1} (A_\beta - \langle A_\beta \rangle) \quad (176)$$

It is worth to mention that these operators are explicitly dependent on the density D . Using this definition, we have $\langle e_\alpha \rangle = \langle e_\beta^\dagger \rangle = 0$ while

$$\langle \langle e_\alpha^\dagger | e_\beta \rangle \rangle = \frac{1}{\sqrt{\lambda_\alpha \lambda_\beta}} (U^{-1} C U)_{\alpha\beta} = \delta_{\alpha\beta} \quad (177)$$

Therefore, couples of operators $(e_\alpha^\dagger, e_\beta)$ are D -independent. We also have the inverse relation

$$A_\alpha - \langle A_\alpha \rangle = \sum_\beta \sqrt{\lambda_\beta} U_{\alpha\beta} e_\beta = \sum_\beta \sqrt{\lambda_\beta} e_\beta^\dagger U_{\beta\alpha}^{-1}, \quad (178)$$

provided that the $\{A_\alpha\}$ are hermitian operators.

Projection of observables: With the aid of eq. (175) and new operators (eq. 176), any observable, denoted by B could be projected onto the subspace of the $\{A_\alpha\}$. Let us now consider a new operator B and assume that it is eventually partially correlated to A_α , the new operator

$$B^\perp = B - \sum_\alpha e_\alpha \langle \langle e_\alpha^\dagger | B \rangle \rangle \quad (179)$$

⁴ It is worth mentioning that the strict equivalent of statistical mechanics would be the symmetric quantity:

$$C'_{\alpha\beta} = \frac{1}{2} \langle A_\alpha A_\beta + A_\beta A_\alpha \rangle - \langle A_\alpha \rangle \langle A_\beta \rangle. \quad (173)$$

Strictly speaking, only the above quantity can be regarded as a scalar product. However, as it will become clear in the following, it is more convenient to define the non-symmetric $C_{\alpha\beta}$.

⁵ Note that the λ_i measure the information content with respect to D of the new operators e_α .

is statistically independent of the $\{A_\alpha\}$ with respect to D (D -independent). First, B^\perp verifies $\langle B^\perp \rangle = \langle B \rangle$, while for any operator e_β^\dagger , we have

$$\langle \langle B^\perp | e_\beta^\dagger \rangle \rangle = \langle \langle B | e_\beta^\dagger \rangle \rangle - \sum_\alpha \langle \langle B | e_\alpha^\dagger \rangle \rangle \langle \langle e_\beta^\dagger | e_\alpha \rangle \rangle = 0 \quad (180)$$

due to $\langle \langle e_\beta^\dagger | e_\alpha \rangle \rangle = \delta_{\alpha\beta}$. Since, the A_α are linear combination of the e_β^\dagger , $\langle \langle B^\perp | A_\alpha \rangle \rangle = 0$ for any α . The new operator can also directly be expressed in terms of the operator A_α , we finally obtain

$$B^\perp = B - \sum_{\alpha\beta} (A_\alpha - \langle A_\alpha \rangle) C_{\alpha\beta}^{-1} \langle \langle A_\beta | B \rangle \rangle, \quad (181)$$

or written differently

$$B = B^\parallel + B^\perp \quad (182)$$

with

$$B^\parallel = \sum_{\alpha\beta} (A_\alpha - \langle A_\alpha \rangle) C_{\alpha\beta}^{-1} \langle \langle A_\beta | B \rangle \rangle. \quad (183)$$

Therefore, using the same technique as the Principal Component Analysis, any operators can be decomposed into two operators, the second one is statistically independent from the observables $\{A_\alpha\}$, while the first one could be written as a linear combination of the $\{A_\alpha\}$ and contains all the information on the correlation between B and the latter observables. Properties of the two operators B^\parallel and B^\perp are:

$$\langle B^\parallel \rangle = 0, \quad \text{and} \quad \langle \langle B^\parallel | A_\alpha \rangle \rangle = \langle \langle B | A_\alpha \rangle \rangle, \quad (184)$$

$$\langle B^\perp \rangle = \langle B \rangle, \quad \text{and} \quad \langle \langle B^\perp | A_\alpha \rangle \rangle = 0, \quad (185)$$

valid for any α . In the limit where B is fully described in the subspace of the $\{A_\alpha\}$, then B^\perp simply identifies with a number $\langle B \rangle$. If on opposite case, B is statistically independent from these observables, $B^\parallel = 0$.

Projection operators: Using the notation $|B\rangle\rangle$, two projectors denoted respectively by \mathbb{P}_A and \mathbb{Q}_A , can be introduced with

$$\begin{aligned} |B^\parallel\rangle\rangle &= \mathbb{P}_A |B\rangle\rangle, \\ |B^\perp\rangle\rangle &= \mathbb{Q}_A |B\rangle\rangle = (1 - \mathbb{P}_A) |B\rangle\rangle, \end{aligned} \quad (186)$$

with the convention

$$\mathbb{P}_A \equiv \sum_\alpha |e_\alpha^\dagger\rangle\rangle \langle \langle e_\alpha^\dagger| = \sum_{\alpha\beta} |A_\alpha\rangle\rangle C_{\alpha\beta}^{-1} \langle \langle A_\beta|. \quad (187)$$

It could be easily checked that $\mathbb{P}_A^2 = \mathbb{P}_A$ and $\mathbb{Q}_A^2 = \mathbb{Q}_A$ and therefore verify standard properties of projectors. The projection onto the subspace of $\{|A\rangle\rangle\}$ is illustrated in figure 12.

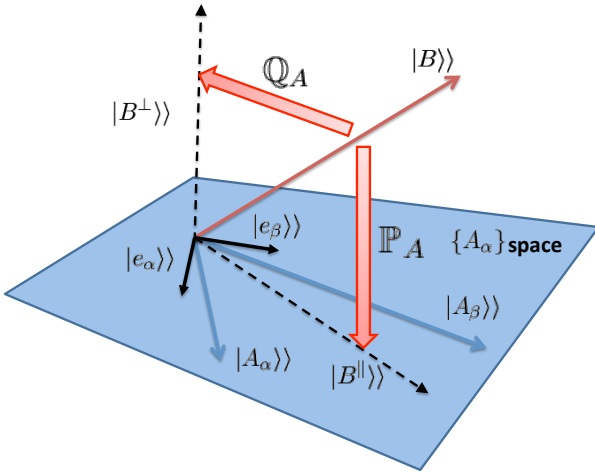


Fig. 12. Schematic representation of the projection technique assuming only two observables (A_α, A_β). Different entities introduced in the text are shown.

C Mean-field as a projected dynamics

As we have seen in section 2, the mean-field approach is a powerful method to select relevant degrees of freedoms (DOF) and provide an optimal evolution of them in the absence of knowledge of others irrelevant DOF at least for short time. It is often said that mean-field theory “corresponds to the optimal projected evolution onto a sub-space of the total observable manifold”. The present appendix goal is to illustrate what is hidden behind this sentence. In section 2.2, we already have shown that variational principle used in combination with variational states given by (9) leads to the exact evolution of the $\{A_\alpha\}$ over short time. It is shown in the present appendix that mean-field evolution corresponds to a projected dynamic onto the subspace of variables $\{A_\alpha\}$ where the projection is nothing but the statistical projection in appendix B.

C.1 Projector associated to mean-field

Trial states given by eq. (9) are not a priori normalized along the path. To enforce normalization, an additional parameter is generally added [27]. Equivalently, one could slightly modify equation (9) as

$$|\mathbf{Q} + \delta\mathbf{Q}\rangle = e^{\sum_{\alpha} \delta q_{\alpha} (A_{\alpha} - \langle A_{\alpha} \rangle)} |\mathbf{Q}\rangle. \quad (188)$$

This automatically insures a constant normalization of the state along the path. Accordingly equation (14) now becomes:

$$i\hbar\langle\mathbf{Q}|(A_\alpha - \langle A_\alpha \rangle)|\dot{\mathbf{Q}}\rangle = \langle\mathbf{Q}|(A_\alpha - \langle A_\alpha \rangle)H|\mathbf{Q}\rangle, (189)$$

where $|\dot{\mathbf{Q}}\rangle$ could be written in terms of the $\{q_\alpha\}$ evolutions as

$$|\dot{\mathbf{Q}}\rangle = \sum_{\alpha} \dot{q}_{\alpha} (A_{\alpha} - \langle A_{\alpha} \rangle) |\mathbf{Q}\rangle. \quad (190)$$

The evolution of \mathbf{Q} given above is nothing but an approximate evolution with an effective Hamiltonian written in terms of a linear combination of the $\{A_\alpha\}$ operators. Combining these equations leads to

$$i\hbar \sum_{\beta} \dot{q}_{\beta} C_{\alpha\beta} = \langle \mathbf{Q} | (A_{\alpha} - \langle A_{\alpha} \rangle) H | \mathbf{Q} \rangle, \quad (191)$$

where C denotes the correlation matrix whose components are defined in eq. (174). Inverting the equation to obtain \dot{q}_α explicitly finally gives:

$$\begin{aligned}
i\hbar|\dot{\mathbf{Q}}\rangle &= \left\{ \sum_{\alpha\beta} (A_\alpha - \langle A_\alpha \rangle) |\mathbf{Q}\rangle C_{\alpha\beta}^{-1} \langle \mathbf{Q}| (A_\beta - \langle A_\beta \rangle) \right\} H |\mathbf{Q}\rangle \\
&= \left\{ \sum_{\alpha\beta} (A_\alpha - \langle A_\alpha \rangle) C_{\alpha\beta}^{-1} \langle \langle A_\beta | H \rangle \rangle \right\} |\mathbf{Q}\rangle \\
&= H^{\parallel}(t) |\mathbf{Q}\rangle.
\end{aligned} \tag{192}$$

Therefore, the mean-field evolution is indeed equivalent to a projected dynamics onto a sub-space containing the relevant information on selected observables. More generally, for any observable that are eventually out of the relevant subspace, mean-field will provide the best approximation retaining only the optimal path for the $\{\langle A_\alpha \rangle\}$ observables. The projected dynamic corresponds to an effective mean-field Hamiltonian, denoted hereafter simply by $H_{\text{MF}}(t)$. This Hamiltonian writes as a linear combination of the $\{A_\alpha\}$ operators and identifies with the projected part of H onto the relevant space. Note that same conclusion can be drawn using a slightly different approach based on Liouville representation [120].

In a pure density case, i.e. $D = |\mathbf{Q}\rangle\langle\mathbf{Q}|$, one can further precise the approximation made by introducing a projector \mathcal{P}_A directly acting in Hilbert space

$$\mathcal{P}_A(t) = \sum_{\alpha\beta} (A_\alpha - \langle A_\alpha \rangle) |\mathbf{Q}\rangle C_{\alpha\beta}^{-1} \langle \mathbf{Q}| (A_\beta - \langle A_\beta \rangle) \quad (193)$$

According to eq. (192), we simply have $H_{\text{MF}}(t) = \mathcal{P}_A(t)H$.

D Mean-field from Thouless theorem

In this appendix, the mean-field equation are deduced by applying the Hamiltonian (31) without the residual interaction term directly to an initial state written as $\prod_{\alpha} a_{\alpha}^{\dagger} |-\rangle$ where $|-\rangle$ is a single-particle vacuum. Using the fact that $e^{-\frac{dt}{i\hbar} H_{MF}} e^{\frac{dt}{i\hbar} H_{MF}} = 1$ and $e^{\frac{dt}{i\hbar} H_{MF}} |-\rangle = |-\rangle$

$$\begin{aligned}
e^{\frac{dt}{i\hbar}H_{MF}}|\Psi\rangle &= e^{\frac{dt}{i\hbar}H_{MF}}\prod_{\alpha}a_{\alpha}^{\dagger}|-\rangle \\
&= e^{\frac{dt}{i\hbar}H_{MF}}a_{\alpha_1}^{\dagger}e^{-\frac{dt}{i\hbar}H_{MF}}e^{\frac{dt}{i\hbar}H_{MF}}a_{\alpha_2}^{\dagger}e^{\frac{dt}{i\hbar}H_{MF}} \\
&\quad \dots e^{-\frac{dt}{i\hbar}H_{MF}}a_{\alpha_N}^{\dagger}e^{-\frac{dt}{i\hbar}H_{MF}}e^{+\frac{dt}{i\hbar}H_{MF}}|-\rangle.
\end{aligned}$$

Considering the transformation of each creation operator separately, we have

$$\begin{aligned} e^{\frac{dt}{i\hbar} H_{MF}} a_{\alpha}^{\dagger} e^{-\frac{dt}{i\hbar} H_{MF}} &= a_{\alpha}^{\dagger} + \frac{dt}{i\hbar} [H_{MF}, a_{\alpha}^{\dagger}] + O(dt) \\ &= a_{\alpha}^{\dagger} + \frac{dt}{i\hbar} \sum_i a_i^{\dagger} \langle i | h[\rho] | \alpha \rangle + O(dt) \\ &\equiv a_{\alpha+d\alpha}^{\dagger} + O(dt), \end{aligned} \quad (194)$$

where the expression of the mean-field operator defined in eq. (31) has been used and where "i" refers to the complete original basis. From the above identity, we see that, the propagated many-body state writes:

$$|\Psi(t+dt)\rangle \propto \prod_{\alpha} a_{\alpha+d\alpha}^{\dagger} |-\rangle, \quad (195)$$

where, using $\sum_i |i\rangle \langle i| = 1$, the single-particle states evolves according to

$$i\hbar \frac{d|\alpha\rangle}{dt} = h[\rho] |\alpha\rangle, \quad (196)$$

which is nothing but the standard mean-field evolution.

E Ito calculus

E.1 Basic rules for Ito stochastic calculation

We are considering a stochastic evolution

$$dx = a(x)dt + b(x)\xi(t)dt \quad (197)$$

which could be integrated as

$$x(t) = x_0 + \int_0^t a(x)dt + \int_0^t b(x)\xi(t)dt. \quad (198)$$

The problem is to define the second integral. We define the stochastic function

$$W(t) = \int_0^t \xi(s)ds \quad (199)$$

The fundamental formula is

$$\begin{aligned} \langle W(t) W(t') \rangle &= \int_0^t \int_0^{t'} \langle \xi(s) \xi(s') \rangle ds ds' \\ &= \int_0^{\min(t,t')} \delta(s-s') ds = \min(t, t'). \end{aligned} \quad (200)$$

Thus, we have

$$dx = a(x)dt + b(x)dW. \quad (201)$$

In the Ito rule for the evaluation of integrals, we define

$$\int G(t) dW = \sum_{i=1}^n G(t_{i-1}) (W(t_i) - W(t_{i-1})). \quad (202)$$

Rules :

$$\begin{cases} dW dW = dt \\ dW^{2+N} = 0 \end{cases}, \quad (203)$$

If f is a function of W such that $f = f(W, t)$, we have the rule $df = \left[\frac{\partial f}{\partial t} + \frac{1}{2} \frac{\partial^2 f}{\partial W^2} \right] dt + \frac{\partial f}{\partial W} dW$.

Example :

$$\begin{aligned} d(\exp(W)) &= \exp(W + dW) - \exp(W) \\ &= \exp(W) (dW + \frac{1}{2} dt). \end{aligned} \quad (204)$$

Correlation formula :

Let $G(t)$ (and $F(t)$) be a non-anticipating function, i.e. a function independent on the future, i.e. independent of $W(s) - W(t)$ if $s > t$. Then, we have the property

$$\left\langle \int_0^t G(s) dW(s) \int_0^t F(s') dW(s') \right\rangle = \int_0^t \langle G(s) F(s) \rangle ds$$

Changing variables : If f depends on a variable x that evolves according to the above stochastic equation, then

$$df[x] = \left\{ a(t) f'(t) + \frac{1}{2} b^2(t) f''(t) \right\} dt + b(t) f'(t) dW.$$

E.2 Differentiation of specific operators

E.2.1 Entropy

We consider the entropy associated to the density D defined as

$$S(D) = -\text{Tr}(D \ln D). \quad (205)$$

In a mean-field approach, since we are considering a specific form for the density along the path, $S(D)$ identifies with the one-particle entropy

$$S(\rho) = -\text{Tr}(\rho \ln(\rho) + (1-\rho) \ln(1-\rho)) \quad (206)$$

Let us derive here the variation of entropy associated with the stochastic one-body density. We start from

$$dS(\rho) = S(\rho + d\rho) - S(\rho). \quad (207)$$

For any operator such that $u^2 = u$, we have

$$d[u \ln u] = du \ln(u) + du - \frac{du^2}{2} + \frac{du^2}{u}. \quad (208)$$

We finally obtain

$$dS(\rho) = -\text{Tr} \left\{ d\rho \ln \left(\frac{1-\rho}{\rho} \right) + d\rho^2 \left[1 - \frac{1}{\rho} - \frac{1}{1-\rho} \right] \right\}$$

Using the fact that $d\rho^2 = 0 + O(dt)$, we finally obtain

$$dS(\rho) = -\text{Tr} \left\{ d\rho \ln \left(\frac{1-\rho}{\rho} \right) \right\} \quad (209)$$

Therefore, the average evolution of $S(\rho)$ is equal to zero.

E.3 evolution of df^{-1}

Expression of df^{-1} : using $f^{-1}f = 1$, we have $df^{-1} \cdot f + f^{-1} \cdot df + df^{-1} \cdot df = 0$, we thus have

$$\begin{aligned} df^{-1} &= -f^{-1} \cdot df \cdot (f + df)^{-1} = -f^{-1} \cdot df \cdot (1 + f^{-1}df)^{-1} f^{-1} \\ &= -f^{-1} \cdot df \cdot f^{-1} + f^{-1} \cdot df \cdot f^{-1} df \cdot f^{-1}. \end{aligned} \quad (210)$$

E.4 Evolution of a determinant

Evolution of $\det(f)$: using

$$\det(f + df) = \det(f) \det(1 + f^{-1}df), \quad (211)$$

and

$$\det(1 + M) = 1 + \text{Tr}(M) - \frac{1}{2} \left(\text{Tr}(M^2) - \text{Tr}(M)^2 \right) + \dots$$

we obtain

$$\begin{aligned} \det(1 + f^{-1}df) &= 1 + \text{Tr}(f^{-1}df) - \frac{1}{2} \{ \text{Tr}(f^{-1}df \cdot f^{-1}df) \\ &\quad - \text{Tr}(f^{-1}df)^2 \}. \end{aligned} \quad (212)$$

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